

Open Notebook Science Challenge

Solubilities

of

Organic Compounds

in

Organic Solvents

Compiled and Measured by:

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Bill Hooker, Postdoctoral Researcher in Molecular Biology
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and

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Preface

The Open Notebook Science Solubility Challenge

Solubility is an important consideration for many chemistry applications. Synthetic chemists usually use a solvent to perform reactions and knowledge of the solubility of the starting materials or products can be very useful to pick an appropriate solvent. Analytical chemists can use solubility to design separation techniques and factor in dynamic range considerations. Physical chemists can create and evaluate their models of how molecules interact in the solubilization and precipitation processes.

Solubility data can be obtained from a variety of online and offline sources. As with all chemical data, it can be a challenge to evaluate reported measurements. Some databases offer no references while others provide citations to peer reviewed journal articles. Given the choice, more weight is generally given to the latter. This is reasonable in most cases because more information about the purity of compounds and the methods used are available in peer-reviewed articles.

However, the information for how a specific measurement was obtained within a journal article is not generally provided. General methods are provided but the raw data for a specific measurement are typically not published. Peer review is not intended to validate individual measurements - its function is to ensure that the authors made appropriate conclusions based on their processed datasets and the state of knowledge in the field.

The Open Notebook Science Challenge was initiated in the fall of 2008 as the result of a discussion on a train in the UK between Jean-Claude Bradley and Cameron Neylon.[1,2] The concept was very simple: create a crowdsourcing opportunity for the chemistry community to contribute solubility measurements under Open Notebook Science conditions. This method of publication entails providing immediate public access to the chemist's laboratory notebook, as well as all raw data used to compute the measurements.[3,4]

On Sept 3, 2008 the first ONSC measurements were recorded by Bradley and Neylon at the University of Southampton in Neylon's laboratory.[5] The project was soon sponsored by Submeta, offering ten \$500 awards for students in the US or the UK who best recorded how they performed their experiments.[6] Furthermore, the first 3 winners also received one year subscriptions to Nature magazine, thanks to a sponsorship from the Nature Publishing Group.[7] Sigma-Aldrich supported the contest by donating chemicals upon request.[8]

Students were evaluated by a group of judges who convened once a month to deliberate the next award. Judges also provided feedback to the students by commenting on their lab notebook pages directly on the wiki. Their expertise ranged from chemistry to mathematics, spectroscopy and molecular biology.

Techniques

Participants in the ONS Challenge were not required to use a specific method to measure solubility - although they were required to properly document their experiments and analyses. Due to its simplicity, most measurements in the past year were made using the SAMS NMR technique, requiring no volume measurement or calibration curves.[9] Two assumptions are made with this method. The first is that the volume of solute and solvent are additive, with the error becoming negligible at low solubility values. The second is that NMR integration values are proportional to the amount of solvent and solute. Some deviations from this have been observed for default NMR parameters and in later experiments long relaxation times are introduced into the protocol (D1 = 50s).[10]

Data Curation

Since an Open Notebook approach is used in this work, those interested in the validity of the measurements can assess the methods used - both for the preparation of saturated solutions and the raw data from the measurements. Over time, values in the database are likely to improve and possibly some errors may be uncovered and corrected. However, on the whole, we feel that the values provided in this work should be of use to chemists trying to gain an appreciation of solubility for most applications. This is especially the case for values that are not obtainable from any other source.

When clearly erroneous data points are discovered, they are flagged in the database as "DONOTUSE". This way interfaces with the dataset can ignore these values while allowing anyone to investigate why the data points were flagged. This might happen when early experiments did not allow for sufficient mixing or NMR D1 relaxation times were long enough to fully integrate peaks of interest. Out of 681 reported measurements, 51 are currently marked in this way. A shared Google Spreadsheet is used to collect and curate the dataset. This allows easy data entry while providing a simple way to interrogate the database for visualization applications via the Google API.[11]

Literature data and format conversions

An additional 400 solubility measurements from the literature are included in the database. These generally correspond to compounds that are structurally identical or similar to the compounds measured by the ONS Challenge participants. These values are averaged in with the values from the participants, with appropriate references provided. In order to compare values, conversions from molar fraction or g solute/100g solvent to molarity were made by assuming that the volumes are additive and obtaining the density of the solutes in most cases from the predicted values in ChemSpider.[12]

For the convenience of chemists with diverse applications, all three formats are provided. For the cases where solutes are miscible with the solvent, the molarity reported is simply the solute's density. The practical interpretation of this is that solutions of any molarity below the solute's density can be prepared.

In the process of converting units and averaging heterogeneous data sources, no attempt has been made to track significant figures. Those interested in any information about the precision of measurements should consult each individual data source.

This may not be an easy task for measurements only carried out once and where factors such as the quality of spectral peaks and baselines are not optimal.

This collection will be most valuable for those who do not require highly precise measurements for their applications. For example, synthetic chemists can easily use rough estimates of solubility to select appropriate solvents for a reaction. In any case, one would be wise to consider all measurements as provisional, regardless of the source. As more data are collected, subsequent editions of this book will adjust values accordingly.

Searching the database

The values in this database can be accessed and filtered in various ways. More information is available at the ONS Challenge wiki[13] and Chapter 16 of the book "Beautiful Data".[14]

Database version

Archived as Excel Spreadsheet by WebCite on December 11, 2009.[15]

References

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- [15] Bradley, Jean-Claude; Lang Andrew. Solubilities Summary Sheet. Open Notebook Science Challenge. 2009-12-11. URL:<http://spreadsheets.google.com/pub?key=plwwufp30hfq0udnEmRD1aQ&output=xls>. Accessed: 2009-12-11. (Archived by WebCite® at <http://www.webcitation.org/5lx5ry3BV>)



Jean-Claude Bradley is an Associate Professor of Chemistry and E-Learning Coordinator for the College of Arts and Sciences at Drexel University. He leads the UsefulChem project, an initiative started in the summer of 2005 to make the scientific process as transparent as possible by publishing all research work in real time to a collection of public blogs, wikis and other web pages. Jean-Claude coined the term Open Notebook Science to distinguish this approach from other more restricted forms of Open Science. Jean-Claude teaches undergraduate organic chemistry courses with most content freely available on public blogs, wikis, games, Second Life and audio and video podcasts. He has a Ph.D. in organic chemistry and has published articles and obtained patents in the areas of synthetic and mechanistic chemistry, gene therapy, nanotechnology and scientific knowledge management. <http://usefulchem.blogspot.com>



Cameron Neylon is a biophysicist who has always worked in interdisciplinary areas and is an advocate of open research practice and improved data management. He currently works as Senior Scientist in Biomolecular Sciences at the ISIS Neutron Scattering facility at the Science and Technology Facilities Council (STFC). Along with his work in structural biology and biophysics his research and writing focuses on the interface of web technology with science and the successful (and unsuccessful) application of generic and specially designed tools in the academic research environment. He is a founder member of the Open Knowledge Foundation Science Working Group and writes regularly on Open Research at his blog, Science in the Open. <http://blog.openwetware.org/scienceintheopen>



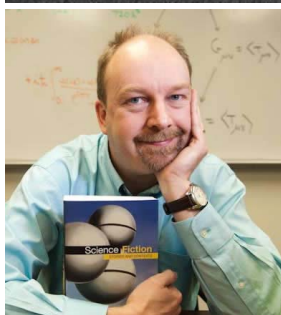
Rajarshi Guha is a Research Scientist at the NIH Chemical Genomics Center (NCGC). At the NCGC he is involved in cheminformatics methodology and software development for various aspects of high throughput screening for small molecules and RNAi. His research makes extensive use of statistical methods and has been applied to a variety of biological systems. Along with algorithm development, he is extensively involved in cheminformatics software development, including development of toolkits, web services and integration of these into distributed infrastructures. As a believer in Open Source and Open Data, much of his research and software is available under Open Source licenses. <http://blog.rguha.net>



Antony Williams is the host of ChemSpider, the online chemistry portal leading the charge towards open and collaborative chemistry. ChemSpider provides access to over 23million unique chemical entities sourced from almost 300 data sources and provides a platform for community based depositions and curation to clean up internet-based chemistry. Antony spent over a decade in the commercial scientific software business as Chief Science Officer for a Cheminformatics software company and during his tenure over saw their product development, marketing and sales teams. He is an accomplished NMR spectroscopist with over 100 peer-reviewed publications. During his career he was the NMR Technology Leader for the Eastman-Kodak company and has worked in both academia and national government research institutions. He has recently taken his passion for providing access to chemistry related information and software services to the masses by hosting the ChemSpider service. <http://www.chemspider.com/blog/>



Bill Hooker is a molecular biologist by trade and has worked on G protein signaling, PCR diagnostics, anti-schistosome vaccines, HIV replication and molecular mechanisms of cancer. He serves as an associate editor on the innovative Open Access journal BioMed Central Research Notes and as a member of the advisory board of the Berglund Center for Internet Studies. He is currently the R&D team leader at a small biotech company in Portland, OR. He has never had an idea that couldn't be improved by sharing it with as many people as possible, and doesn't believe that anyone else has, either. He is particularly interested in extending the "open" ethos of Open Source software and Open Access publishing to all aspects of science, from raw data to hypothesis testing by way of distributed, collaborative effort. <http://www.sennoma.net>



Andrew Lang is a Professor of Mathematics at Oral Roberts University. His PhD training is in the area of quantum field theory in curved spacetime. While remaining active in this area he has always enjoyed working collaboratively on interdisciplinary projects ranging from modeling basketball free throws to the stability of spinning spacecraft under thrust. His interests include the relationship between science and science fiction and the epistemological differences between teleology and metaphysical naturalism. As a result of being a judge for the Open Notebook Science Challenge he has developed an appreciation for openness in science, multi-dimensional data visualization and cheminformatics. http://webapps.oru.edu/new_php/blog/index.php?user_id=23

Educational Partners



J. Brent Friesen from Dominican University incorporated the Open Notebook Science Solubility Challenge into his Sophomore Organic Chemistry laboratory course in January 2009. He has been a professor in the natural science department at Dominican University since 1999. He regularly teaches Organic Chemistry (lecture and laboratory), Biochemistry, Introduction to Organic Chemistry, Chemistry of Natural Products, and Forensic Chemistry. His research focuses on the automation of countercurrent separation technology, anti-tuberculosis compounds, and interactions with Reichardt's Dye. Friesen has also done research with undergraduates on projects such as "Biorenewable Solvents for Countercurrent Chromatography" and "Used Coffee Grounds: A New Source of Biofuels." Friesen is a regular volunteer with the Oak Park Education Foundation's Global Village, a program matching scientists with elementary school classrooms. His recent articles include "Saying What You Mean: Teaching Mechanisms in Organic Chemistry" (Journal of Chemical Education) and "Countercurrent Separation of Natural Products" (Journal of Natural Products).

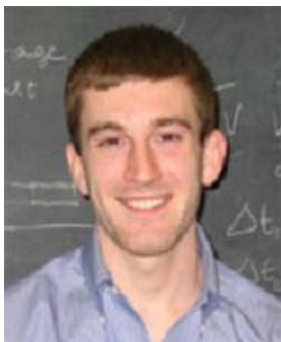
Students



Tim Bohinski (April 2009 Submeta Award winner) is a senior at Drexel University majoring in chemistry, with a strong interest in organic and theoretical chemistry. He will be graduating with a B.S. in June 2010. He is currently performing undergraduate research in the theoretical/physical field, studying nanoparticle optics, specifically in the area of plasmoms. He plans to continue his studies at the doctorate level. Tim is also a member of the Drexel American Chemical Society and was a member of the Drexel Crew Team. In my spare time he enjoys the outdoors, staying fit, and homebrewing. LinkedIn profile: <http://www.linkedin.com/pub/timothy-bohinski/18/110/a7> Supervisor: Jean-Claude Bradley, Drexel



David Bulger (February 2009 Submeta Award winner) is a junior Chemistry major at Oral Roberts University in Tulsa, OK. Since freshman year, he has been involved in research ranging from water purity, red tide in Second Life, collaboration between water utilities and academia, NMR solubility determination and Sortase A inhibition. After his undergraduate degree, he plans to pursue an M.D. or M.D./Ph.D. http://biolab.isis.rl.ac.uk/david_bulger. Supervisor: Robert Stewart, Oral Roberts University



Matthew Federici (June 2009 Submeta Award winner) graduated from the University of Virginia in 2008. After receiving the Naval ROTC Tweeddale Scholarship Award in 2004, Matthew studied naval nuclear engineering and interned on the USS Alexandria. As a varsity student athlete, he doubled majored in mechanical engineering as well as aerospace engineering. Matthew spent his senior year at UVa studying biomechanics under Dr. Pradip Sheth. His undergraduate academic career finished by winning the Cyrus Society Award, given to a select few of student athletes with outstanding academic performance and community service. Matthew is pursuing his PhD in Mechanical Engineering under Dr. Minjun Kim at Drexel University. As a GAANN fellow, he is currently investigating biomimetics and drug delivery systems. Matthew plans to attend medical school following the completion of his dissertation. Website: <http://microfluidics.tripod.com/> Supervisor: Jean-Claude Bradley, Drexel



Jennifer (Jenny) Hale (December 2008 Submeta Award winner) gained a BSc in Chemistry with Pharmacology from the University of Southampton, UK, in 2004. Following her degree she spent 15 months working on the synthesis of phosphoramidites before taking up a PhD in the department of chemical biology in 2006. Jenny's area of research for her PhD has been the directed evolution of a beta-glucuronidase into a beta-galactosidase via neutral drift, a phenomenon found in natural evolution that has only recently begun to be explored in laboratory evolution. Additionally, her research has been used in the development and testing of an electronic laboratory notebook in the form of a blog: LaBLog (http://blogs.chem.soton.ac.uk/neutral_drift) as well as wider investigations into Open Notebook Science. Outside of the laboratory, Jenny is a keen ballroom and latin dancer and spent a year as president of the Southampton University Ballroom and Latin Dance Society, as well as competing in numerous university dancesport competitions. **Supervisor: Cameron Neylon, Southampton**



Jenna Mancinelli (September 2009 Submeta Award winner) is currently a junior at Drexel University, studying Biology. She is particularly interested in human physiology and its relation to clinical medicine. She hopes to attend medical school following her graduation from Drexel University. In her spare time, Jenna enjoys going to concerts, studying Italian and experimenting with her culinary skills. **Supervisor: Jean-Claude Bradley, Drexel**



Khalid Baig Mirza (January 2009 Submeta Award winner) obtained a BSc in Chemistry and Biology from Osmania University, India. He earned an MS in Chemistry from Fairleigh Dickinson University at Madison, NJ in 2002. He is currently working towards a PhD at Drexel University under the guidance of Prof. Jean-Claude Bradley. His research focuses on the synthesis of potentially active anti-malarial diamides obtained from a Ugi reaction. His research is performed in the open as 'Open Notebook Science'. He enjoys gardening, cricket and keeping up to date on world affairs. **Supervisor: Jean-Claude Bradley, Drexel**



Marshall Moritz (July 2009 Submeta Award winner) is a junior at Syracuse University with a double major in chemistry and math. **Supervisor: Jean-Claude Bradley, Drexel**



Daniel Rein (August 2009 Submeta Award winner) is currently a student studying chemistry and biology at Drexel University. He plays guitar in Jazz Band and is passionate about music. For freshman year he studied physics at Northeastern. <http://www.linkedin.com/pub/daniel-rein/18/31a/72b> **Supervisor: Jean-Claude Bradley, Drexel**



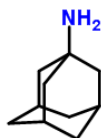
Cedric Tchakounte (March 2009 Submeta Award winner) is a senior majoring in Biological Sciences & Biotechnology at Drexel University. He is a distinguished student, having received multiple Dean's List honors and the Who's Who Among Students in American Universities & Colleges award. He has also shown his dedication to community and service by being a mentor for Guided Youths. He enjoys performing research, because he believes it to be a cornerstone to learning true science. With his academic chapter as an undergraduate coming to an end, Cedric looks forward to what awaits. He plans on pursuing a career in medicine. **Supervisor: Jean-Claude Bradley, Drexel**



Hai Truong (December 2009 Submeta Award winner) is pursuing a BS in Chemistry at Drexel University from 2009. After graduating with honors from a high school for the Gifted in Vietnam, he came to the United States for college. In 2008, he attended Collin College in McKinney, TX. At Collin, he was a member of Phi Theta Kappa, an international honor society for two-year colleges. In 2009, he transferred to Drexel University with a Dean's Scholarship. Beside academic studies, Hai enjoys swimming and playing tennis. **Supervisor: Jean-Claude Bradley, Drexel**

Solubilities

1-adamantylamine $C_{10}H_{17}N^{14}$



Compound Data

Molecular weight	151.249	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	2.22
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.066 g/cm ³
SMILES	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>				
InChIKey	DKNWSYNQZKUICI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.82	0.05	17.99
methanol	0.36	0.02	7.62

1-octadecylamine $C_{18}H_{39}N^{69}$



Compound Data

Molecular weight	269.509	H bond acceptors	1	Rule of 5 violations	1
Compound type	amine	H bond donors	2	ACD/ALogP	8.37
Phase 25°C	solid	Rotatable bonds	17	Predicted density	0.818 g/cm ³
SMILES	<chem>NCCCCCCCCCCCCCCCCC</chem>				
InChIKey	REYJJPSVUYRZGE-UHFFFAOYSA-N				

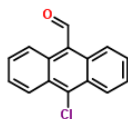
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.08	0.00	2.96
ethanol	1.77	0.20	146.72
methanol	1.68	0.14	134.67
THF	1.68	0.23	112.18
toluene	1.34	0.20	74.24

10-chloro-9-anthraldehyde $C_{15}H_9ClO^{57}$

Compound Data

Molecular weight	240.684	H bond acceptors	1	Rule of 5 violations	0
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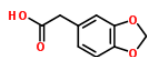


Compound type	aldehyde	H bond donors	0	ACD/ALogP	4.7
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.327 g/cm ³
SMILES	<chem>O=Cc1cc(Cl)cc([N+](=O)[O-])cc1</chem>				
InChIKey	SHYBXXMECBHHFH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.00	0.00	0.00
THF	0.08	0.01	2.16

2-(1,3-benzodioxol-5-yl)acetic acid C₉H₈O₄^{98, 82}

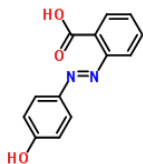


Compound Data					
Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.406 g/cm ³
SMILES	<chem>O=C(O)Cc1ccc2OCOc2cc1</chem>				
InChIKey	ODVLMCWNGKLROU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.67	0.04	17.68
DMSO	5.37	0.55	282.22
THF	2.73	0.25	83.68

2-(4-hydroxyphenyl-azo)benzoic acid C₁₃H₁₀N₂O₃^{3, 32}



Compound Data					
Molecular weight	242.23	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	3.72
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.3 g/cm ³
SMILES	<chem>O=C(O)c1cc(N=Nc2ccc(O)cc2)ccc1</chem>				
InChIKey	DWQOTEPNRWVUDA-CCEZHUSRSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.09	0.01	2.68
methanol	0.06	0.00	1.95
THF	0.55	0.05	16.42

2-chloro-5-nitrobenzaldehyde C₇H₄ClNO₃^{69, 105, 208, 33, 205}



Compound Data					
Molecular weight	185.565	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.5
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.485 g/cm ³
SMILES	<chem>O=Cc1cc(Cl)cc([N+](=O)[O-])cc1</chem>				
InChIKey	VFVHWCKUHAEDMY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.31	0.15	80.47
chloroform	2.9	0.27	56.27
DMSO	2.93	0.25	78.05
ethanol	*	*	*
methanol	*	*	*
THF	2.79	0.25	87.80
toluene	1.74	0.19	47.44

* This aldehyde reacts with alcohols to form a hemiacetal.

2-chloro-5-nitrobenzoic acid $C_7H_4ClNO_4$ ⁹⁰⁵



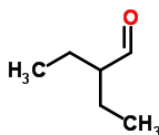
Compound Data

Molecular weight	201.564	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.02
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.602 g/cm ³
SMILES	<chem>O=C(O)c1cc(ccc1Cl)[N+](=O)[O-]</chem>				
InChIKey	QUEKGYQTRJVEQC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.78	0.07	21.66
1-decanol	0.39	0.07	9.98
1-heptanol	0.54	0.08	14.24
1-hexanol	0.64	0.08	17.19
1-octanol	0.48	0.07	12.51
1-pentanol	0.74	0.08	20.28
1-propanol	0.95	0.08	27.36
2-butanol	0.91	0.09	25.86
2-methyl-1-propanol	0.63	0.06	17.22
2-methyl-2-propanol	1.21	0.12	35.78
2-pentanol	0.76	0.08	20.94
2-propanol	1.13	0.09	33.57
3-methyl-1-butanol	0.68	0.07	18.53
butyl acetate	0.46	0.06	11.11
dibutyl ether	0.1	0.02	2.62
diethyl ether	0.57	0.06	16.86
diisopropyl ether	0.19	0.03	5.18
ethanol	1.4	0.09	43.91
ethyl acetate	0.75	0.08	18.59
methyl acetate	0.89	0.08	22.25
pentyl acetate	0.43	0.06	10.39
THF	2.97	0.27	105.73

2-ethylbutyraldehyde $C_6H_{12}O$ ²²



Compound Data

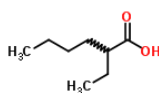
Molecular weight	100.159	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.79
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.799 g/cm ³
SMILES	<chem>O=CC(CC)CC</chem>				
InChIKey	UNNGUFMVYQJGTD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.13	□	□

□ Solute is very soluble/miscible, conversion fail.

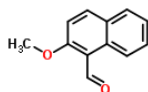
2-ethylhexanoic acid C₈H₁₆O₂²²



Compound Data			
Molecular weight	144.211	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.72
Phase 25°C	liquid	Rotatable bonds	5 Predicted density 0.926 g/cm ³
SMILES	O=C(O)C(CC)CCCC		
InChIKey	OBETXYAYXDNJHR-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.26	0.91	4777.15

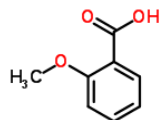
2-methoxy-1-naphthaldehyde C₁₂H₁₀O₂²⁰⁵



Compound Data			
Molecular weight	186.207	H bond acceptors	2 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.95
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.169 g/cm ³
SMILES	O=Cc1c2c(ccc1OC)cccc2		
InChIKey	YIQLTKAOHRZOL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	1.26	0.06	38.98

2-methoxybenzoic acid C₈H₈O₃^{905, 34}

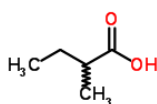


Compound Data			
Molecular weight	152.147	H bond acceptors	3 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.5
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.207 g/cm ³
SMILES	O=C(O)c1ccccc1OC		
InChIKey	ILUJQPXNXACGAN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.57	0.05	11.61
1-decanol	0.22	0.04	4.16
1-heptanol	0.34	0.05	6.59
1-hexanol	0.37	0.05	7.24
1-octanol	0.3	0.05	5.76
1-pentanol	0.47	0.05	9.37
1-propanol	0.76	0.06	16.09
1,4-dioxane	1.53	0.14	28.99
2-butanol	0.5	0.05	10.14
2-ethyl-1-hexanol	0.25	0.04	4.78
2-methyl-1-butanol	0.39	0.04	7.71
2-methyl-1-pentanol	0.35	0.04	6.84
2-methyl-1-propanol	0.41	0.04	8.21
2-methyl-2-propanol	0.53	0.05	10.75
2-pentanol	0.39	0.04	7.71
2-propanol	0.59	0.05	12.26

3-methyl-1-butanol	0.36	0.04	7.09
4-methyl-2-pentanol	0.32	0.04	6.26
butyl acetate	0.34	0.04	6.10
chloroform	0.47	0.04	5.01
dibutyl ether	0.04	0.01	0.78
diethyl ether	0.24	0.02	5.13
diisopropyl ether	0.06	0.01	1.21
ethanol	1.19	0.08	27.31
ethyl acetate	5.63	0.66	328.57
methanol	1.82	0.09	47.72
methyl acetate	0.86	0.07	16.16
pentyl acetate	0.26	0.04	4.64
propylene carbonate	0.99	0.13	14.28
THF	2.02	0.18	45.61

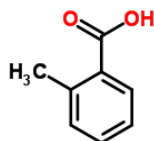
2-methyl butyric acid C₅H₁₀O₂²²



Compound Data			
Molecular weight	102.132	H bond acceptors	2
Compound type	carboxylic acid	Rule of 5 violations	0
Phase 25°C	liquid	H bond donors	1
SMILES	O=C(O)C(C)CC	ACD/ALogP	1.13
InChIKey	WLAMNBDJUVNPJU-UHFFFAOYSA-N	Rotatable bonds	2
		Predicted density	0.962 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.16	0.93	4515.12

2-methylbenzoic acid C₈H₈O₂⁹⁰⁵

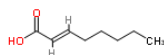


Compound Data			
Molecular weight	136.148	H bond acceptors	2
Compound type	carboxylic acid	Rule of 5 violations	0
Phase 25°C	solid	H bond donors	1
SMILES	O=C(O)c1ccccc1C	ACD/ALogP	2.36
InChIKey	ZWLPBLYKEWSWPD-UHFFFAOYSA-N	Rotatable bonds	1
		Predicted density	1.151 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	1.61	0.15	33.64
1-decanol	1.04	0.18	19.50
1-heptanol	1.28	0.18	25.04
1-hexanol	1.38	0.17	27.52
1-octanol	1.16	0.18	22.24
1-pentanol	1.49	0.16	30.37
1-propanol	1.77	0.14	38.34
1,4-dioxane	2.64	0.25	52.53
2-butanol	1.75	0.17	37.51
2-methyl-1-butanol	1.25	0.14	24.69
2-methyl-1-propanol	1.28	0.12	25.64
2-methyl-2-propanol	2.19	0.21	50.05
2-pentanol	1.68	0.19	35.28
2-propanol	1.95	0.16	43.63
3-methyl-1-butanol	1.34	0.15	26.80
4-methyl-2-pentanol	1.39	0.17	27.93
butyl acetate	1.17	0.15	20.87
dibutyl ether	0.58	0.09	10.87

diethyl ether	1.65	0.17	38.03
diisopropyl ether	0.86	0.11	17.20
ethanol	2.08	0.14	48.15
ethyl acetate	1.49	0.15	27.42
methyl acetate	1.51	0.13	27.56
pentyl acetate	1.04	0.15	18.31
propylene carbonate	0.46	0.06	5.50
THF	2.92	0.26	67.18

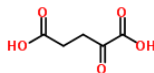
2-octenoic acid C₈H₁₄O₂²²



Compound Data			
Molecular weight	142.196	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.93
Phase 25°C	liquid	Rotatable bonds	5 Predicted density 0.955 g/cm ³
SMILES	O=C(O)/C=C/CCCC		
InChIKey	CWMPPVPFLSZGCY-VOTSOKGWSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.64	0.96	11068.64

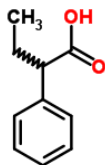
2-oxopentanedioic acid C₅H₆O₅²⁵



Compound Data			
Molecular weight	146.098	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP -1.43
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.499 g/cm ³
SMILES	O=C(O)C(=O)CCC(=O)O		
InChIKey	KPGXRSRHYNQIFN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	2.99	0.20	79.04
methanol	5.02	0.29	190.70
THF	3.12	0.26	72.46

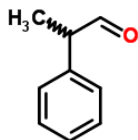
2-phenylbutyric acid C₁₀H₁₂O₂^{79, 83}



Compound Data			
Molecular weight	164.201	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.38
Phase 25°C	solid	Rotatable bonds	3 Predicted density 1.09 g/cm ³
SMILES	O=C(O)C(c1ccccc1)CC		
InChIKey	OFJWFSNDPCAWDK-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	6.18	0.83	1968.04
DMSO	5.97	0.81	886.12
ethanol	6.2	0.85	1977.18
THF	5.96	0.82	1059.60
toluene	5.35	0.74	519.73

2-phenylpropanal C₉H₁₀O²¹



Compound Data

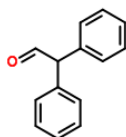
Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.13
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	0.98 g/cm ³
SMILES	<chem>c1ccccc1C(C)C=O</chem>				
InChIKey	IQVAERDLDAZARL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.53	□	□

□ Solute is very soluble/miscible, conversion fail.

2,2-diphenylacetaldehyde C₁₄H₁₂O²¹



Compound Data

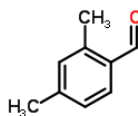
Molecular weight	196.245	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	3.67
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	1.069 g/cm ³
SMILES	<chem>c1ccccc1C(c1ccccc1)C(=O)</chem>				
InChIKey	HLLGFGBLKOIZOM-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	5.64	□	□

□ Solute is very soluble/miscible, conversion fail.

2,4-dimethylbenzaldehyde C₉H₁₀O²¹



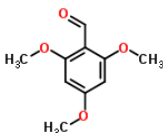
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.56
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.003 g/cm ³
SMILES	<chem>O=Cc1cc(C)cc1C</chem>				
InChIKey	GISVICWQYMUPJF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.17	0.88	3128.10

2,4,6-trimethoxybenzaldehyde C₁₀H₁₂O₄⁸²



Compound Data

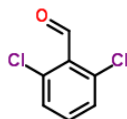
Molecular weight	196.2	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.49
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.133 g/cm ³
SMILES	<chem>O=Cc1c(OC)cc(OC)cc1OC</chem>				
InChIKey	CRBZVDLXAIFERF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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THF 0.14 0.01 3.11

2,6-dichlorobenzaldehyde C₇H₄Cl₂O^{208, 205}



Compound Data

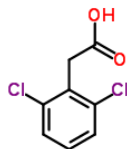
Molecular weight	175.012	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	3.03
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.4 g/cm ³
SMILES	<chem>O=Cc1c(Cl)cccc1Cl</chem>				
InChIKey	DMIYKWPEFRFTPY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.35	0.08	38.05
chloroform	3.41	0.32	69.35
ethanol	*	*	*
methanol	*	*	*
THF	2.48	0.22	69.58
toluene	1.74	0.19	44.68

* This aldehyde reacts with alcohols to form a hemiacetal.

2,6-dichlorophenylacetic acid C₈H₆Cl₂O₂^{82, 85}



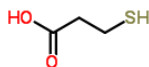
Compound Data

Molecular weight	205.038	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.71
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.456 g/cm ³
SMILES	<chem>Clc1cccc(Cl)c1CC(=O)O</chem>				
InChIKey	SFAILOOQFZNOAU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	3.03	0.30	120.05

3-mercaptopropionic acid C₃H₆O₂S²²



Compound Data

Molecular weight	106.144	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.43
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	1.223 g/cm ³
SMILES	<chem>C(CS)C(=O)O</chem>				
InChIKey	DKIDEFUBRARXTE-UHFFFAOYSA-N				

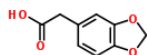
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.48	0.99	44306.20

3,4-(methylenedioxy)phenylacetic acid C₉H₈O₄¹³⁸

Compound Data

Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.406 g/cm ³

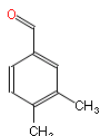


SMILES O=C(O)Cc1ccc2OCOc2c1
InChIKey ODVLMCWNGKLROU-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.1	0.01	2.44

3,4-dimethylbenzaldehyde C₉H₁₀O⁵⁹



Compound Data

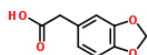
Molecular weight 134.175 **H bond acceptors** 1 **Rule of 5 violations** 0
Compound type aldehyde **H bond donors** 0 **ACD/ALogP** 2.56
Phase 25°C liquid **Rotatable bonds** 1 **Predicted density** 1.003 g/cm³
SMILES Cc1ccc(cc1C)C=O
InChIKey POQJHLBMLVTHAU-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.54	□	□
methanol	7.54	□	□
THF	7.54	□	□

□ Solute is very soluble/miscible, conversion fail.

3,4-methylenedioxyphenylacetic acid C₉H₈O₄^{129, 132, 131}

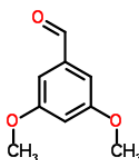


Molecular weight 180.157 **H bond acceptors** 4 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 1 **ACD/ALogP** 1.37
Phase 25°C solid **Rotatable bonds** 2 **Predicted density** 1.406 g/cm³
SMILES O=C(O)Cc1ccc2OCOc2c1
InChIKey ODVLMCWNGKLROU-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.55	0.03	13.67
methanol	0.94	0.04	25.57
THF	1.95	0.17	51.81

3,5-dimethoxybenzaldehyde C₉H₁₀O₃^{205, 208}



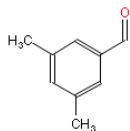
Molecular weight 166.174 **H bond acceptors** 3 **Rule of 5 violations** 0
Compound type aldehyde **H bond donors** 0 **ACD/ALogP** 1.53
Phase 25°C solid **Rotatable bonds** 3 **Predicted density** 1.114 g/cm³
SMILES O=Cc1cc(OC)cc(OC)c1
InChIKey VFZRZRDOXPRTSC-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
methanol	1.71	0.09	50.66
THF	4.03	0.45	185.73

3,5-dimethylbenzaldehyde C₉H₁₀O⁶³



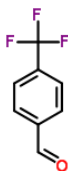
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.56
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.003 g/cm ³
SMILES	<chem>Cc1cc(C=O)cc(C)c1</chem>				
InChIKey	NBEFMISJJNGCIZ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p _{ph} (g/100g)
ethanol	7.44	0.99	27092.92
methanol	7.44	0.99	28064.38
THF	7.44	0.99	23376.63

4-(trifluoromethyl)benzaldehyde C₈H₅F₃O²¹



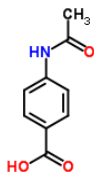
Compound Data

Molecular weight	174.12	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.61
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.293 g/cm ³
SMILES	<chem>c1cc(C=O)ccc1C(F)(F)F</chem>				
InChIKey	BEOBZEOPTQQELP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p _{ph} (g/100g)
methanol	7.32	0.96	11867.65

4-acetamidobenzoic acid C₉H₉NO₃¹³⁷



Compound Data

Molecular weight	179.173	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	1.31
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.326 g/cm ³
SMILES	<chem>O=C(Nc1ccc(cc1)C(=O)O)C</chem>				
InChIKey	QCXJEYYXVJIFCE-UHFFFAOYSA-N				

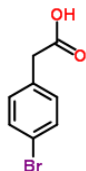
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p _{ph} (g/100g)
acetonitrile	0.01	0.00	0.24
benzene	0.00	0.00	0.00
ethanol	0.23	0.01	5.45
methanol	0.19	0.01	4.64
THF	0.17	0.01	3.45

4-bromophenylacetic acid C₈H₇BrO₂⁸⁵

Compound Data

Molecular weight	215.044	H bond acceptors	2	Rule of 5 violations	0
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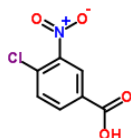


Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.28
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.616 g/cm ³
SMILES	<chem>Brc1ccc(cc1)CC(=O)O</chem>				
InChIKey	QOWSWEBLNVACCL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	3.68	0.37	171.85

4-chloro-3-nitrobenzoic C₇H₄ClNO₄⁹⁰⁵



Compound Data

Molecular weight	201.564	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.602 g/cm ³
SMILES	<chem>O=[N+]([O-])c1cc(ccc1Cl)C(=O)O</chem>				
InChIKey	DFXQXFGFOLXAPO-UHFFFAOYSA-N				

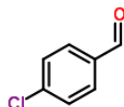
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.31	0.03	8.08
1-decanol	0.19	0.04	4.74
1-heptanol	0.25	0.04	6.34
1-hexanol	0.27	0.03	6.90
1-octanol	0.23	0.04	5.80
1-pentanol	0.27	0.03	6.95
1-propanol	0.37	0.03	9.84
1,4-dioxane	1.43	0.13	35.32
2-butanol	0.32	0.03	8.39
2-ethyl-1-hexanol	0.15	0.02	3.75
2-methyl-1-pentanol	0.19	0.02	4.82
2-methyl-1-propanol	0.19	0.02	4.90
2-methyl-2-propanol	0.38	0.04	10.01
2-pentanol	0.3	0.03	7.77
2-propanol	0.39	0.03	10.45
3-methyl-1-butanol	0.24	0.03	6.17
4-methyl-2-pentanol	0.23	0.03	5.89
butyl acetate	0.23	0.03	5.39
dibutyl ether	0.05	0.01	1.30
diethyl ether	0.24	0.02	6.80
diisopropyl ether	0.1	0.01	2.69
ethanol	0.55	0.03	15.27
ethyl acetate	0.36	0.04	8.46
methyl acetate	0.44	0.04	10.34
methyl butyrate	0.21	0.02	4.88
pentyl acetate	0.16	0.02	3.73
propyl acetate	0.26	0.03	6.08
propylene carbonate	0.15	0.02	2.56
THF	1.95	0.17	57.61

4-chlorobenzaldehyde C₇H₅ClO^{7, 209}

Compound Data

Molecular weight	140.567	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.21

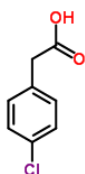


Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.243 g/cm ³
SMILES	<chem>O=Cc1ccc(Cl)cc1</chem>				
InChIKey	AVPYQKSLYISFPO-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	5.59	0.45	285.27
chloroform	3.61	0.33	57.17
ethanol	2.81	0.20	74.23
methanol	3.55	0.20	110.72
THF	5.29	0.51	204.25

4-chlorophenylacetic acid C₈H₇ClO₂^{4, 75, 73}



Compound Data

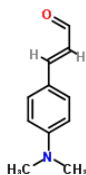
Molecular weight	170.593	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.1
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.324 g/cm ³
SMILES	<chem>Clc1ccc(cc1)CC(=O)O</chem>				
InChIKey	CDPKJZJVTHSESZ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.67	0.10	48.72
DMSO	5.74	0.61	342.14
methanol	7.76	□	□
THF	4.45	0.45	197.18
toluene	0.89	0.10	19.69

□ Solute is very soluble/miscible, conversion fail.

4-dimethylamino cinnamaldehyde C₁₁H₁₃NO^{3, 32}



Compound Data

Molecular weight	175.227	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.63
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.057 g/cm ³
SMILES	<chem>O=CC=Cc1ccc(N(C)C)cc1</chem>				
InChIKey	RUKJCCIJLIMGEP-ONEGZZNKSA-N				

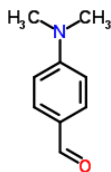
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.06	0.00	1.25
methanol	0.07	0.00	1.65
THF	0.42	0.03	8.75

4-dimethylaminobenzaldehyde C₉H₁₁NO^{208, 205}

Compound Data

Molecular weight	149.19	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.81
Phase 25°C	solid	Rotatable bonds	2	Predicted density	3



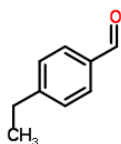
SMILES O=Cc1ccc(N(C)C)cc1
InChIKey BGNGWHSBYQYVRX-UHFFFAOYSA-N

1.072 g/cm

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.6	0.18	81.37
chloroform	4.02	0.42	90.76
ethanol	0.63	0.04	13.21
methanol	1.36	0.07	33.24
THF	2.5	0.23	63.27
toluene	1.54	0.17	33.57

4-ethylbenzaldehyde C₉H₁₀O⁶³



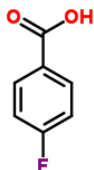
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.63
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.001 g/cm ³
SMILES	<chem>CCc1ccc(C=O)cc1</chem>				
InChIKey	<chem>QNGNSVIICDLXHT-UHFFFAOYSA-N</chem>				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.3	0.95	5840.38
methanol	7.3	0.94	6049.80
THF	7.3	0.96	5039.27

4-fluorobenzoic acid C₇H₅FO₂^{106, 121}



Compound Data

Molecular weight	140.112	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.07
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.319 g/cm ³
SMILES	<chem>O=C(O)c1ccc(F)cc1</chem>				
InChIKey	<chem>BBYDXOIZLAWGSL-UHFFFAOYSA-N</chem>				

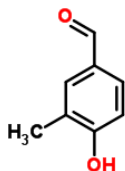
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.39	0.02	7.63
DMSO	4.19	0.35	96.26
ethanol	0.8	0.05	15.71
methanol	0.76	0.03	15.38
THF	2.49	0.21	52.47
toluene	0.00	0.00	0.00

4-hydroxy-3-methylbenzaldehyde C₈H₈O₂⁵⁷

Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.85

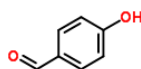


Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.175 g/cm ³
SMILES	<chem>O=Cc1cc(O)c(c1)C</chem>				
InChIKey	BAKYASSDAXQKKY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	2.15	0.14	49.98
methanol	2.78	0.15	74.15
THF	3.05	0.27	71.04

4-hydroxybenzaldehyde C₇H₆O₂^{208, 57, 205, 58, 85, 88}

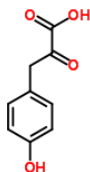


Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.226 g/cm ³
SMILES	<chem>O=Cc1ccc(O)cc1</chem>				
InChIKey	RGHHSNMVTDWUBI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.46	0.09	27.93
chloroform	1.75	0.14	17.26
ethanol	2.53	0.17	52.82
methanol	3.4	0.18	83.19
THF	3.7	0.32	79.10
toluene	0.02	0.00	0.28

4-hydroxyphenylpyruvic acid C₉H₈O₄¹⁵

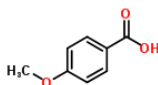


Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	-0.2
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.397 g/cm ³
SMILES	<chem>c1cc(O)ccc1CC(=O)C(=O)O</chem>				
InChIKey	KKADPXVIOXHVKI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.05
methanol	0.91	0.04	24.67

4-methoxybenzoic acid C₈H₈O₃⁹⁰⁵

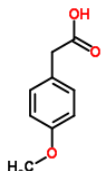


Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.96
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.207 g/cm ³
SMILES	<chem>COc1ccc(cc1)C(=O)O</chem>				
InChIKey	ZEYHEAKUIGZSGI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.12	0.01	2.30
1-decanol	0.07	0.01	1.30
1-heptanol	0.09	0.01	1.69
1-hexanol	0.1	0.01	1.89
1-octanol	0.08	0.01	1.49
1-pentanol	0.1	0.01	1.90
1-propanol	0.13	0.01	2.53
1,4-dioxane	0.39	0.04	6.27
2-butanol	0.13	0.01	2.51
2-ethyl-1-hexanol	0.07	0.01	1.31
2-methyl-1-propanol	0.08	0.01	1.54
2-methyl-2-propanol	0.17	0.02	3.29
2-propanol	0.14	0.01	2.74
3-methyl-1-butanol	0.08	0.01	1.52
butyl acetate	0.08	0.01	1.39
dibutyl ether	0.02	0.00	0.39
diethyl ether	0.09	0.01	1.89
diisopropyl ether	0.03	0.00	0.60
ethanol	0.2	0.01	4.00
ethyl acetate	0.13	0.01	2.24
pentyl acetate	0.06	0.01	1.04
THF	0.7	0.06	12.92

4-methoxyphenylacetic acid C₉H₁₀O₃^{89, 136, 92}



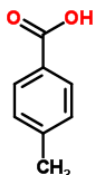
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.42
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.179 g/cm ³
SMILES	O=C(O)Cc1ccc(OC)cc1				
InChIKey	NRPFNQUDKRYCNX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.23	0.15	72.11
DMSO	4.5	0.47	186.41
methanol	2.5	0.14	85.19
THF	3.32	0.33	114.38
toluene	0.37	0.04	7.45

4-methylbenzoic acid C₈H₈O₂^{2, 25}



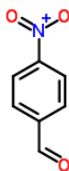
Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.36
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.151 g/cm ³
SMILES	O=C(O)c1ccc(C)cc1				
InChIKey	LPNBBFKOUUSUDB-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.78	0.05	14.89
methanol	0.78	0.04	15.54
THF	1.61	0.14	29.84

4-nitrobenzaldehyde $C_7H_5NO_3$ ^{904, 98, 111, 212, 33, 205, 82, 122}



Compound Data

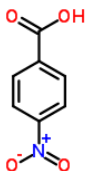
Molecular weight	151.12	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.56
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.338 g/cm ³
SMILES	<chem>c1cc(C=O)ccc1[N+](=O)[O-]</chem>				
InChIKey	BXRFSQSNOROATLV-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	*	*	*
1-propanol	*	*	*
2-propanol	*	*	*
acetonitrile	1.13	0.07	26.16
benzene	0.46	0.04	8.40
carbon tetrachloride	0.07	0.01	0.63
chloroform	1.02	0.08	11.57
cyclohexane	0.01	0.00	0.19
dichloromethane	1.29	0.09	18.23
DMF	1.68	0.15	36.02
DMSO	1.24	0.09	19.83
ethanol	*	*	*
ethylene glycol	*	*	*
methanol	*	*	*
THF	0.88	0.07	16.33
toluene	0.46	0.05	8.42

* This aldehyde reacts with alcohols to form a hemiacetal.

4-nitrobenzoic acid $C_7H_5NO_4$ ⁹⁰⁵



Compound Data

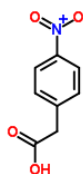
Molecular weight	167.119	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.89
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.468 g/cm ³
SMILES	<chem>O=[N+]([O-])c1ccc(C(=O)O)cc1</chem>				
InChIKey	OTLNPYWUJOZPPA-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.09	0.01	1.89
1-decanol	0.05	0.01	1.01
1-heptanol	0.08	0.01	1.65
1-hexanol	0.08	0.01	1.65
1-octanol	0.06	0.01	1.23
1-pentanol	0.09	0.01	1.87
1-propanol	0.11	0.01	2.34
1,4-dioxane	0.47	0.04	8.34
2-butanol	0.1	0.01	2.11
2-methyl-1-butanol	0.05	0.01	1.04
2-methyl-1-pentanol	0.05	0.01	1.03
2-methyl-1-propanol	0.07	0.01	1.47
2-methyl-2-butanol	0.17	0.02	3.57
2-methyl-2-propanol	0.15	0.01	3.17
2-pentanol	0.08	0.01	1.67
2-propanol	0.11	0.01	2.35

3-methyl-1-butanol	0.07	0.01	1.46
4-methyl-2-pentanol	0.07	0.01	1.45
butyl acetate	0.08	0.01	1.52
dibutyl ether	0.02	0.00	0.43
diethyl ether	0.1	0.01	2.30
diisopropyl ether	0.03	0.00	0.66
ethanol	0.14	0.01	3.05
ethyl acetate	0.13	0.01	2.46
methanol	0.18	0.01	4.08
methyl acetate	0.14	0.01	2.62
pentyl acetate	0.05	0.01	0.95
propylene carbonate	0.06	0.01	0.84
THF	0.78	0.06	15.82

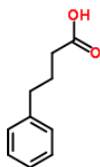
4-nitrophenylacetic acid C₈H₇NO₄¹⁵



Compound Data			
Molecular weight	181.145	H bond acceptors	5
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	3
SMILES	<chem>c1cc(CC(=O)O)ccc1[N+](=O)[O-]</chem>		
InChIKey	YBADLXQNJCMBKR-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.15
methanol	1.29	0.06	37.21

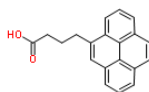
4-phenylbutyric acid C₁₀H₁₂O₂⁷²



Compound Data			
Molecular weight	164.201	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	4
SMILES	<chem>O=C(O)CCCC1=CC=CC=C1</chem>		
InChIKey	OBKXEAXTFZPCHS-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.19	0.02	3.94
chloroform	3.99	0.44	108.74
diethyl ether	4.02	0.51	226.42
methanol	4.54	0.38	310.15
toluene	4.06	0.52	195.66

4-pyrenebutanoic acid C₂₀H₁₆O₂^{61, 99, 51, 24, 30, 84, 91}



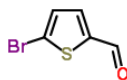
Compound Data			
Molecular weight	288.34	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	4
SMILES	<chem>O=C(O)CCCC4=CC=CC=C1C=CC3C(C12)C4=CC=C3C12</chem>		
InChIKey	GSBSDUZVSCTUKA-UHFFFAOYSA-N		

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.06	0.00	2.22
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.03	0.00	0.58
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.07	0.00	1.64
diethyl ether	0.02	0.00	0.79
DMF	1.88	0.21	107.11
DMSO	2.07	0.21	100.37
ethanol	0.06	0.00	2.25
hexane	0.00	0.00	0.00
methanol	0.01	0.00	0.51
THF	0.55	0.05	19.99
toluene	0.00	0.00	0.00

5-bromothiophene-2-carbaldehyde C₅H₃BrOS²¹

Compound Data



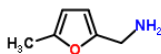
Molecular weight	191.046	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.97
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.789 g/cm ³
SMILES	C1=C(SC(=C1)Br)C=O				
InChIKey	GFBVUFQNLUCPX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.22	0.96	15186.93

5-methylfurfurylamine C₆H₉NO²⁶

Compound Data



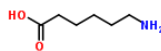
Molecular weight	111.142	H bond acceptors	2	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	0.71
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.024 g/cm ³
SMILES	o1c(ccc1CN)C				
InChIKey	YSEAGSCGERFGBL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.97	0.94	5010.81

6-aminocaproic acid C₆H₁₃NO₂¹⁴

Compound Data

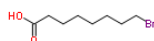


Molecular weight	131.173	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	3	ACD/ALogP	-0.11
Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.042 g/cm ³
SMILES	C(CCC(=O)O)CCN				
InChIKey	SLXKOJJOQWFEFD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.06	0.00	1.05

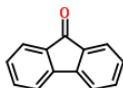
8-bromooctanoic acid C₈H₁₅BrO₂^{3, 66}



Compound Data			
Molecular weight	223.107	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.76
Phase 25°C	solid	Rotatable bonds	7 Predicted density 1.324 g/cm ³
SMILES	BrCCCCCCCC(=O)O		
InChIKey	BKJFDZSBZWHRNH-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	4.07	0.43	370.56
methanol	3.28	0.24	217.27
THF	3.56	0.42	219.59

9-fluorenone C₁₃H₈O⁹⁰⁵

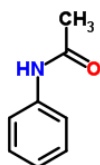


Compound Data			
Molecular weight	180.202	H bond acceptors	1 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	0 ACD/ALogP 3.58
Phase 25°C	solid	Rotatable bonds	0 Predicted density 1.244 g/cm ³
SMILES	O=C3c1ccccc1c2c3ccccc2		
InChIKey	YLQWCDOCJODRMT-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.37	0.03	8.75
1-decanol	0.42	0.08	9.73
1-heptanol	0.43	0.06	10.08
1-hexanol	0.41	0.05	9.63
1-octanol	0.43	0.07	10.04
1-pentanol	0.41	0.05	9.69
1-propanol	0.38	0.03	9.12
2-butanol	0.33	0.03	7.80
2-ethyl-1-hexanol	0.35	0.06	8.09
2-methyl-1-pentanol	0.36	0.05	8.41
2-methyl-1-propanol	0.25	0.02	5.84
2-methyl-2-butanol	0.4	0.04	9.43
2-methyl-2-propanol	0.31	0.03	7.27
2-pentanol	0.35	0.04	8.21
2-propanol	0.29	0.02	6.90
2,2,4-trimethylpentane	0.07	0.01	1.80
3-methyl-1-butanol	0.31	0.03	7.23
4-methyl-2-pentanol	0.29	0.04	6.73
acetonitrile	1.57	0.10	49.02
benzene	2.61	0.27	86.63
butyronitrile	1.93	0.19	61.50
carbon tetrachloride	1.83	0.18	26.44
cyclohexane	0.15	0.02	3.50
cyclooctane	0.17	0.02	3.98
cyclopentanol	0.82	0.07	16.70
decane	0.12	0.02	3.00

dibutyl ether	0.37	0.06	9.03
dichloromethane	4.03	0.40	139.36
diethyl ether	0.88	0.09	24.76
diisopropyl ether	0.37	0.05	9.29
ethanol	3.08	0.25	128.48
heptane	0.11	0.02	2.90
hexadecane	0.12	0.03	2.85
hexane	0.1	0.01	2.71
methanol	0.37	0.02	9.36
methyl tert-butyl ether	0.76	0.09	20.52
methylcyclohexane	0.14	0.02	3.32
nonane	0.12	0.02	3.04
octane	0.11	0.02	2.83
propionitrile	1.99	0.17	65.35
tert-butylcyclohexane	0.12	0.02	2.71
toluene	2.17	0.25	65.48
undecane	0.12	0.03	2.96

acetanilide C₈H₉NO³⁵



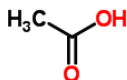
Compound Data

Molecular weight	135.163	H bond acceptors	2	Rule of 5 violations	0
Compound type	amide	H bond donors	1	ACD/ALogP	1.08
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.103 g/cm ³
SMILES	O=C(Nc1ccccc1)C				
InChIKey	FZERHIULMFGESH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	1.42	0.11	30.10

acetic acid C₂H₄O₂²²



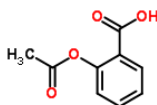
Compound Data

Molecular weight	60.052	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	-0.29
Phase 25°C	liquid	Rotatable bonds	0	Predicted density	1.068 g/cm ³
SMILES	O=C(O)C				
InChIKey	QTBSBXVTEAMEQO-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	17.47	0.98	7876.42

acetylsalicylic acid C₉H₈O₄^{72, 34, 903}



Compound Data

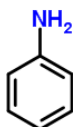
Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.29 g/cm ³
SMILES	O=C(Oc1ccccc1C(=O)O)C				
InChIKey	BSYNYRMUTXBXSQ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
1-hexanol	0.00	0.00	0.00
chloroform	0.18	0.01	2.24
diethyl ether	0.17	0.02	4.27
methanol	1.3	0.06	38.00
toluene	0.00	0.00	0.00

aniline C₆H₇N²⁹



Compound Data

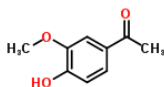
Molecular weight	93.1265	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	0.94
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.015 g/cm ³
SMILES	Nc1ccccc1				
InChIKey	PAYRUJLWNCNPSJ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.97	□	□

□ Solute is very soluble/miscible, conversion fail.

apocynin C₉H₁₀O₃⁹⁰⁶



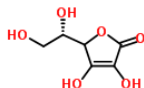
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.158 g/cm ³
SMILES	Oc1ccc(cc1OC)C(C)=O				
InChIKey	DFYRUELUNQRZTB-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.32	0.02	7.01
1,2-dichloroethane	0.41	0.04	6.17
butanone	0.66	0.06	15.41
toluene	0.06	0.01	1.15

ascorbic acid C₆H₈O₆⁷²



Compound Data

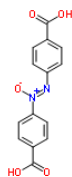
Molecular weight	176.124	H bond acceptors	6	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	4	ACD/ALogP	†
Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.954 g/cm ³
SMILES	O\C1=C(/O)C(=O)O[C@@H](O)[C@H](O)CO				
InChIKey	CIWBBSHSHKDKBQ-JLAZNSOCSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

† ACD/ALogP prediction fail.

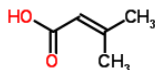
azoxydibenzoic acid C₁₄H₁₀N₂O₅⁷²



Compound Data			
Molecular weight	286.24	H bond acceptors	7 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 4.05
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.41 g/cm ³
SMILES	<chem>O=C(O)c2ccc([N+](=O)[O-])=N/c1ccc(cc1)C(=O)O</chem>		
InChIKey	ZYVHVVGJGLOEKD-NXVVXOECSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

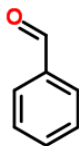
B,B-dimethylacrylic acid C₅H₈O₂¹³⁶



Compound Data			
Molecular weight	100.116	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.35
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.01 g/cm ³
SMILES	<chem>O=C(O)C(=C)C</chem>		
InChIKey	YYPNJNDODFVZLE-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	4.73	0.27	118.40

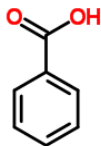
benzaldehyde C₇H₆O²¹



Compound Data			
Molecular weight	106.122	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 1.64
Phase 25°C	liquid	Rotatable bonds	1 Predicted density 1.049 g/cm ³
SMILES	<chem>c1ccccc1C=O</chem>		
InChIKey	HUMNYLRZRPJDN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.85	0.99	39374.95

benzoic acid C₇H₆O₂^{37, 902, 58, 5, 43, 136, 9, 900}

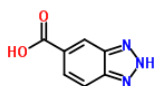


Compound Data			
Molecular weight	122.121	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.9
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.197 g/cm ³
SMILES	<chem>c1ccccc1C(=O)O</chem>		
InChIKey	WPYMKLBDIGXBTP-UHFFFAOYSA-N		

Solubility Data	
Concentration	

Solvent	(M)	Mole Fraction (X)	pph (g/100g)
acetone	1.35	0.11	24.77
acetonitrile	0.76	0.04	13.37
benzene	0.48	0.04	7.06
chloroform	1.8	0.15	17.95
ethanol	2.52	0.17	53.18
methanol	2.84	0.15	64.89
THF	3.37	0.29	69.27
toluene	0.65	0.07	9.81
water	0.03	0.00	0.37

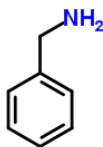
benzotriazole-5-carboxylic acid $C_7H_5N_3O_2$ ^{3, 32}



Compound Data			
Molecular weight	163.133	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.82
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.617 g/cm ³
SMILES	O=C(O)c1ccc2nnnc2c1		
InChIKey			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.04	0.00	0.73
methanol	0.04	0.00	0.76
THF	0.02	0.00	0.36

benzylamine C_7H_9N ²⁹

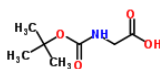


Compound Data			
Molecular weight	107.153	H bond acceptors	1 Rule of 5 violations 0
Compound type	amine	H bond donors	2 ACD/ALogP 1.09
Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.979 g/cm ³
SMILES	NCc1ccccc1		
InChIKey	WGQKYBSKWIADBV-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.16	□	□

□ Solute is very soluble/miscible, conversion fail.

boc-glycine $C_7H_{13}NO_4$ ^{143, 71, 207, 116, 133, 135}

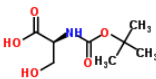


Compound Data			
Molecular weight	175.182	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.75
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.159 g/cm ³
SMILES	O=C(OC(C)(C)C)NCC(=O)O		
InChIKey	VRPJIFMKZZEXLR-UHFFFAOYSA-N		

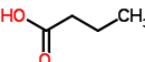
Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	3.63	0.38	177.58
acetonitrile	2.46	0.18	91.84
benzene	0.26	0.02	5.32

chloroform	3.85	0.42	107.55
dichloromethane	4.14	0.43	154.79
diethyl ether	2.65	0.31	105.51
DMSO	4.78	0.55	274.57
ethanol	4.11	0.39	243.70
hexane	0.25	0.03	6.74
methanol	4.73	0.41	384.60
THF	3.72	0.40	164.41
toluene	0.19	0.02	3.93

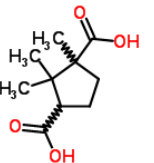
boc-serine C₈H₁₅NO₅^{98, 85}

Compound Data						
	Molecular weight	205.208	H bond acceptors	6	Rule of 5 violations	0
	Compound type	boc serine	H bond donors	3	ACD/ALogP	0.22
	Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.24 g/cm ³
	SMILES	O=C(OC(C)(C)C)N[C@H](C(=O)O)CO				
	InChIKey	FHOAKXBXYSJBGX-YFKPBYRVSA-N				
Solubility Data						
Solvent	Concentration (M)	Mole Fraction (X)		pph (g/100g)		
methanol	3.62	0.28		246.06		
THF	3.11	0.34		145.78		

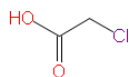
butyric acid C₄H₈O₂²²

Compound Data					
	Molecular weight	88.1051	H bond acceptors	2 Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	1 ACD/ALogP	0.78
	Phase 25°C	liquid	Rotatable bonds	2 Predicted density	0.987 g/cm³
	SMILES	CCCC(=O)O			
	InChIKey	FERIUCNNQJTOY-UHFFFAOYSA-N			
Solubility Data					
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)		
methanol	10.94	0.95	5462.12		

camphoric acid C₁₀H₁₆O₄⁹⁰²

Compound Data						
	Molecular weight	200.232	H bond acceptors	4	Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	1.47
	Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.177 g/cm ³
	SMILES	O=C(O)C1CCC(C(=O)O)(C)C1(C)C				
	InChIKey	LSPHULWDVZXLIL-UHFFFAOYSA-N				
Solubility Data						
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)			
1-propanol	1.72	0.16	61.24			
methanol	2.75	0.18	137.41			

chloroacetic acid C₂H₃ClO₂⁹⁵



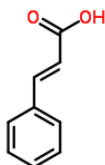
Molecular weight	94.497	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	†
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.398 g/cm ³
SMILES	CICC(O)=O				
InChIKey	FOCAUTSVDIKZOP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	12.45	0.81	993.98
DMSO	11.2	0.77	396.40
methanol	9.45	0.53	328.30
THF	9.63	0.69	288.10
toluene	1.41	0.14	16.95

† ACD/ALogP prediction fail.

cinnamic acid C₉H₈O₂^{72, 902, 48}

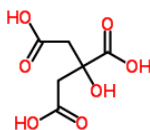


Compound Data					
Molecular weight	148.159	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.41
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.184 g/cm ³
SMILES	O=C(O)\C=C\c1ccccc1				
InChIKey	WBYWAXJHAXSJNI-VOTSOKGWSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.93	0.08	10.40
diethyl ether	0.43	0.04	9.17
ethanol	0.86	0.05	18.31
methanol	1.1	0.05	25.19
toluene	0.3	0.03	5.30

citric acid anhydrous C₆H₈O₇^{902, 25}



Compound Data					
Molecular weight	192.124	H bond acceptors	7	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	4	ACD/ALogP	-1.72
Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.762 g/cm ³
SMILES	O=C(O)CC(O)(C(=O)O)CC(=O)O				
InChIKey	KRKNYBCHXYNGOX-UHFFFAOYSA-N				

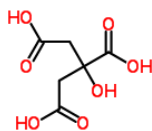
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.00	0.00	0.00
ethanol	1.6	0.10	47.74
methanol	3.08	0.16	118.32
THF	1.8	0.15	47.60

citric acid monohydrate C₆H₈O₇²

Compound Data

Molecular weight	192.124	H bond acceptors	7	Rule of 5 violations	0
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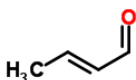


Compound type	carboxylic acid	H bond donors	4	ACD/ALogP	-1.72
Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.762 g/cm ³
SMILES	<chem>O=C(O)CC(O)(C(=O)O)CC(=O)O</chem>				
InChIKey	KRKNYBCHXYNGOX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	1.78	0.12	54.40
methanol	2.27	0.11	76.97
THF	1.52	0.13	38.72

crotonaldehyde C₄H₆O²¹



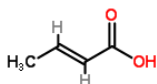
Molecular weight	70.0898	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	0.51
Phase 25°C	solid	Rotatable bonds	1	Predicted density	0.819 g/cm ³
SMILES	<chem>CC=CC=O</chem>				
InChIKey	MLUCVPSAIODCQM-NSCUHMNNSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	12.17	□	□

□ Solute is very soluble/miscible, conversion fail.

crotonic acid C₄H₆O₂^{64, 62}



Molecular weight	86.0892	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.8
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.039 g/cm ³
SMILES	<chem>O=C(O)/C=C/C</chem>				
InChIKey	LDHQCZJRKDOVOX-NSCUHMNNSA-N				

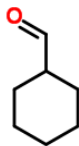
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	3.59	0.22	58.89
benzene	4.45	0.39	69.51
chloroform	7.34	0.60	107.51
DMSO	7.76	0.61	170.26
ethanol	6.15	0.43	138.41
hexane	1.07	0.13	14.97
methanol	7.62	0.47	236.33
THF	8.09	0.66	233.69
toluene	3.52	0.34	49.12

cyclohexanecarbaldehyde C₇H₁₂O²¹

Compound Data

Molecular weight	112.17	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.9
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	



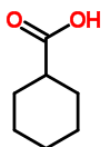
SMILES C1CCC(CC1)C=O
InChIKey KVFDFBHBWTVID-UHFFFAOYSA-N

0.992 g/cm

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.29	0.85	1972.34

cyclohexanecarboxylic acid C₇H₁₂O₂²²

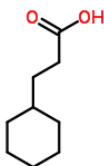


Compound Data
Molecular weight 128.169 H bond acceptors 2 Rule of 5 violations 0
Compound type carboxylic acid H bond donors 1 ACD/ALogP 1.77
Phase 25°C liquid Rotatable bonds 1 Predicted density 1.079 g/cm³
SMILES C1CCC(CC1)C(=O)O
InChIKey NZNMSOFKMUBTKW-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.06	0.89	3220.96

cyclohexanepropionic acid C₉H₁₆O₂²²

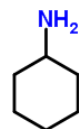


Compound Data
Molecular weight 156.222 H bond acceptors 2 Rule of 5 violations 0
Compound type carboxylic acid H bond donors 1 ACD/ALogP 2.84
Phase 25°C liquid Rotatable bonds 3 Predicted density 1.006 g/cm³
SMILES C1CCC(CC1)CCC(=O)O
InChIKey HJZLEGIHUQJBA-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	5.84	0.73	1301.33

cyclohexylamine C₆H₁₃N²⁹

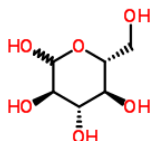


Compound Data
Molecular weight 99.1741 H bond acceptors 1 Rule of 5 violations 0
Compound type amine H bond donors 2 ACD/ALogP 1.4
Phase 25°C liquid Rotatable bonds 1 Predicted density 0.869 g/cm³
SMILES NC1CCCCC1
InChIKey PAFZNILMFXTMIY-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.74	0.99	45092.19

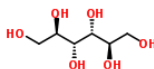
D-glucose C₆H₁₂O₆^{1, 207}



Compound Data			
Molecular weight	180.156	H bond acceptors	6 Rule of 5 violations 1
Compound type	non-Ugi related	H bond donors	5 ACD/ALogP -1.88
Phase 25°C	solid	Rotatable bonds	6 Predicted density 1.732 g/cm ³
SMILES	O[C@H]1[C@H](O)[C@H](OC(O)[C@H]1O)CO		
InChIKey	WQZGKKKJUFFOK-GASJEMHNSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.04	0.00	0.84
THF	0.02	0.00	0.30

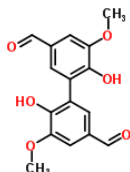
D-mannitol C₆H₁₄O₆^{1, 207}



Compound Data			
Molecular weight	182.172	H bond acceptors	6 Rule of 5 violations 1
Compound type	non-Ugi related	H bond donors	6 ACD/ALogP -4.67
Phase 25°C	solid	Rotatable bonds	11 Predicted density 1.596 g/cm ³
SMILES	O[C@H]1([C@H](O)CO)[C@H](O)[C@H](O)CO		
InChIKey	FBPFZTCFMRRESA-KVTDHHQDSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.01	0.00	0.24
THF	0.02	0.00	0.30

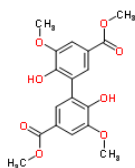
dehydrodivanillin C₁₆H₁₄O₆⁹⁰⁶



Compound Data			
Molecular weight	302.279	H bond acceptors	6 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	2 ACD/ALogP 1.57
Phase 25°C	solid	Rotatable bonds	7 Predicted density 1.356 g/cm ³
SMILES	O=Cc2cc(c1cc(cc(OC)c1O)C=O)c(O)c(OC)c2		
InChIKey	NSTQUZVZBUTVPY-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

di(methyl vanillate) C₁₈H₁₈O₈⁹⁰⁶

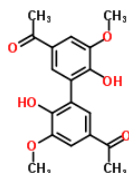


Compound Data			
Molecular weight	362.331	H bond acceptors	8 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	2 ACD/ALogP 2.27
Phase 25°C	solid	Rotatable bonds	9 Predicted density 1.315 g/cm ³
SMILES	O=C(OC)c2cc(c1cc(cc(OC)c1O)C(=O)OC)c(O)c(OC)c2		
InChIKey	DBUKZZKLTUXIQM-UHFFFAOYSA-N		

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.01	0.00	0.31
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

diapocynin C₁₈H₁₈O₆⁹⁰⁶



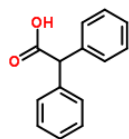
Compound Data

Molecular weight	330.332	H bond acceptors	6	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	2	ACD/ALogP	1.97
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.257 g/cm ³
SMILES	<chem>O=C(c2cc(c1cc(cc(OC)c1O)C(=O)C)c(O)c(OC)c2)C</chem>				
InChIKey	HLNDPICGHQGSU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

diphenylacetic acid C₁₄H₁₂O₂^{81, 77}



Compound Data

Molecular weight	212.244	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	3.25
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.174 g/cm ³
SMILES	<chem>O=C(O)C(c1ccccc1)c2ccccc2</chem>				
InChIKey	PYHXGXCGESYPCW-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.46	0.03	14.26
DMSO	2.56	0.25	92.04
ethanol	1.15	0.08	39.51
methanol	1.27	0.07	46.47
THF	2.91	0.33	144.17
toluene	0.17	0.02	4.27

formic acid CH₂O₂²²



Compound Data

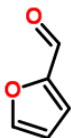
Molecular weight	46.0254	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	-0.54
Phase 25°C	liquid	Rotatable bonds	0	Predicted density	1.154 g/cm ³
SMILES	<chem>O=CO</chem>				
InChIKey	BDAGIHXWWSANSR-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	26.5	□	□

□ Solute is very soluble/miscible, conversion fail.

furfuraldehyde C₅H₄O₂²⁰



Compound Data

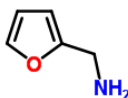
Molecular weight	96.0841	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	0.73
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.145 g/cm ³
SMILES	<chem>O=Cc1ccco1</chem>				
InChIKey	HYBBIBNJHNGZAN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	12.02	□	□

□ Solute is very soluble/miscible, conversion fail.

furfurylamine C₅H₇NO²⁶



Compound Data

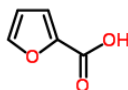
Molecular weight	97.1152	H bond acceptors	2	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	0.25
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.053 g/cm ³
SMILES	<chem>o1c(ccc1)CN</chem>				
InChIKey	DDRPCXLAQZKBJP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.32	□	□

□ Solute is very soluble/miscible, conversion fail.

furoic acid C₅H₄O₃¹⁰⁴



Compound Data

Molecular weight	112.084	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.64
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.322 g/cm ³
SMILES	<chem>OC(=O)c1ccco1</chem>				
InChIKey	SMNDYUVBFMFKNZ-UHFFFAOYSA-N				

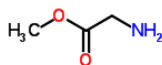
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.1	0.06	18.14
DMSO	6.64	0.52	154.95
methanol	4.12	0.21	94.36
THF	4.07	0.33	77.05
toluene	0.06	0.01	0.78

glycine methyl ester C₃H₇NO₂²⁰⁷

Compound Data

Molecular weight	89.0932	H bond acceptors	3	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	-0.83
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.045 g/cm ³

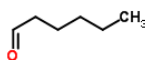


SMILES O=C(OC)CN
InChIKey KQSSATDQUYCRGS-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.19	0.01	2.21
methanol	1.32	0.06	17.60
THF	0.04	0.00	0.40

hexanaldehyde $C_6H_{12}O$ ²¹



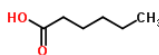
Compound Data
Molecular weight 100.159 **H bond acceptors** 1 **Rule of 5 violations** 0
Compound type aldehyde **H bond donors** 0 **ACD/ALogP** 1.97
Phase 25°C liquid **Rotatable bonds** 4 **Predicted density** 0.801 g/cm³
SMILES CCCCCC=O
InChIKey JARKCYVAAOWBJS-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.33	□	□

□ Solute is very soluble/miscible, conversion fail.

hexanoic acid $C_6H_{12}O_2$ ²²

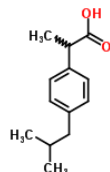


Compound Data
Molecular weight 116.158 **H bond acceptors** 2 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 1 **ACD/ALogP** 1.84
Phase 25°C liquid **Rotatable bonds** 4 **Predicted density** 0.95 g/cm³
SMILES CCCCCC(=O)O
InChIKey FUZZWVXGSFPDMH-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.98	0.93	5071.51

ibuprofen $C_{13}H_{18}O_2$ ⁹⁰⁵



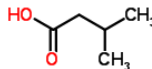
Compound Data
Molecular weight 206.281 **H bond acceptors** 2 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 1 **ACD/ALogP** 3.72
Phase 25°C solid **Rotatable bonds** 4 **Predicted density** 1.029 g/cm³
SMILES O=C(O)C(c1ccc(cc1)CC(C)C)C
InChIKey HEFNWSXXWATRW-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-decanol	1.12	0.22	35.98

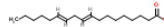
1-octanol	1.2	0.20	39.60
1-pentanol	1.46	0.18	52.50
1-propanol	1.52	0.14	56.72
2-butanol	1.78	0.20	71.27
2-methyl-1-propanol	1.76	0.20	70.04
2-propanol	2.22	0.23	104.32
ethanol	1.18	0.08	40.88
methanol	1.16	0.06	41.41

isovaleric acid C₅H₁₀O₂²²

Compound Data			
	Molecular weight	102.132	H bond acceptors 2 Rule of 5 violations 0
	Compound type	carboxylic acid	H bond donors 1 ACD/ALogP 1.13
	Phase 25°C	liquid	Rotatable bonds 2 Predicted density 0.962 g/cm ³
	SMILES	CC(C)CC(=O)O	
	InChIKey	GWYFCOCPABKNJV-UHFFFAOYSA-N	

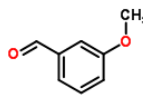
Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.06	0.91	3222.50

linoleic acid C₁₈H₃₂O₂²²

Compound Data			
	Molecular weight	280.445	H bond acceptors 2 Rule of 5 violations 1
	Compound type	carboxylic acid	H bond donors 1 ACD/ALogP 7.18
	Phase 25°C	liquid	Rotatable bonds 14 Predicted density 0.911 g/cm ³
	SMILES	CCCCC=CCC=CCCCCCCC(=O)O	
	InChIKey	OYHQOLUKZRVURQ-AVQMFATSA-N	

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	3.22	0.94	13712.82

m-anisaldehyde C₈H₈O₂²¹

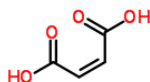
Compound Data			
	Molecular weight	136.148	H bond acceptors 2 Rule of 5 violations 0
	Compound type	aldehyde	H bond donors 0 ACD/ALogP 1.65
	Phase 25°C	liquid	Rotatable bonds 2 Predicted density 1.088 g/cm ³
	SMILES	COc1cc(C=O)ccc1	
	InChIKey	WMPDAIZRQDCGFH-UHFFFAOYSA-N	

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.2	□	□

□ Solute is very soluble/miscible, conversion fail.

maleic acid C₄H₄O₄^{39, 40}

Compound Data			
Molecular weight	116.072	H bond acceptors 4	Rule of 5 violations 0

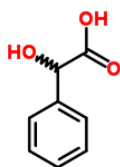


Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	-0.01
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.499 g/cm ³
SMILES	<chem>C(=CC(=O)O)C(=O)O</chem>				
InChIKey	VZCYOOQTPOCHFL-OWOJBTEDSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.41	0.21	68.95
methanol	3.82	0.19	83.62

mandelic acid C₈H₈O₃^{72, 71}

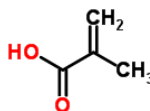


Compound Data					
Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	0.92
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.321 g/cm ³
SMILES	<chem>O=C(O)C(O)c1ccccc1</chem>				
InChIKey	IWYDHOAUDWTVEP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.12	0.01	1.23
diethyl ether	0.77	0.08	17.51
methanol	3.54	0.20	120.77
toluene	0.00	0.00	0.00

methacrylic acid C₄H₆O₂²²

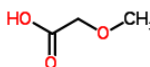


Compound Data					
Molecular weight	86.0892	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.83
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.023 g/cm ³
SMILES	<chem>CC(=C)C(=O)O</chem>				
InChIKey	CERQOIWHTDAKMF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.79	0.98	17218.73

methoxyacetic acid C₃H₆O₃²²



Compound Data					
Molecular weight	90.0779	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	-0.96
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.139 g/cm ³
SMILES	<chem>COCC(=O)O</chem>				
InChIKey	RMIODHQZRUFFFF-UHFFFAOYSA-N				

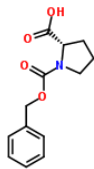
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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methanol 13.03 □ □

□ Solute is very soluble/miscible, conversion fail.

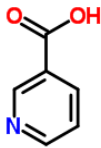
N-Cbz-L-p roline C₁₃H₁₅NO₄¹³⁴



Compound Data			
Molecular weight	249.262	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.17
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.309 g/cm ³
SMILES	O=C(O)[C@H]2N(C(=O)OCc1ccccc1)CCC2		
InChIKey	JXGVXCZADZNAMJ-NSHDSACASA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	4.26	0.49	746.90

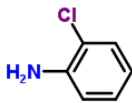
nicotinic acid C₆H₅NO₂^{100, 137}



Compound Data			
Molecular weight	123.109	H bond acceptors	3 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 0.15
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.293 g/cm ³
SMILES	O=C(O)c1ccncc1		
InChIKey	PVNIIMVLHYAWGP-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
DMSO	0.57	0.04	6.71
ethanol	0.09	0.01	1.43
methanol	0.06	0.00	1.03
THF	0.06	0.00	0.75
toluene	0.00	0.00	0.00

o-chloroaniline C₆H₆ClN²⁹

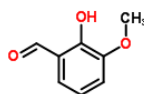


Compound Data			
Molecular weight	127.572	H bond acceptors	1 Rule of 5 violations 0
Compound type	amine	H bond donors	2 ACD/ALogP 1.91
Phase 25°C	liquid	Rotatable bonds	1 Predicted density 1.23 g/cm ³
SMILES	Nc1ccccc1Cl		
InChIKey	AKCROHQIUBRMN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.51	0.97	11802.88

o-vanillin C₈H₈O₃^{208, 205}

Compound Data			
Molecular weight	152.147	H bond acceptors	3 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	1 ACD/ALogP 1.4

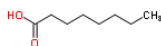


Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm ³
SMILES	<chem>Oc1c(cccc1OC)C=O</chem>				
InChIKey	JJVNINGBHGBWJH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.56	0.17	76.28
ethanol	3.04	0.22	94.99
methanol	2.27	0.12	63.75
THF	5.37	0.56	268.76
toluene	3.82	0.43	126.41

octanoic acid C₈H₁₆O₂²²



Compound Data					
Molecular weight	144.211	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.9
Phase 25°C	liquid	Rotatable bonds	6	Predicted density	0.929 g/cm ³
SMILES	<chem>CCCCCCCC(=O)O</chem>				
InChIKey	WWZKQHOCKIZLMA-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.31	0.93	5899.86

octylamine C₈H₁₉N²⁹

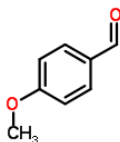


Compound Data					
Molecular weight	129.243	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	3.06
Phase 25°C	liquid	Rotatable bonds	7	Predicted density	0.786 g/cm ³
SMILES	<chem>NCCCCCCCC</chem>				
InChIKey	IOQPZZOEVZRBK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.05	0.98	20005.33

p-anisaldehyde C₈H₈O₂²¹



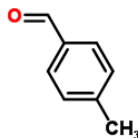
Compound Data					
Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.7
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.088 g/cm ³
SMILES	<chem>COc1ccc(C=O)cc1</chem>				
InChIKey	ZRSNZINYAWTAHE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.22	□	□

□ Solute is very soluble/miscible, conversion fail.

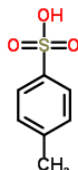
p-tolualdehyde C₈H₈O²¹



Compound Data					
Molecular weight	120.148	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.1
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.023 g/cm³
SMILES	O=Cc1ccc(C)cc1				
InChIKey	FXLOVSHXALFLKQ-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.47	0.99	25859.25

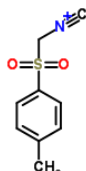
p-toluenesulfonic acid C₇H₈O₃S^{107, 136}



Compound Data					
Molecular weight	172.202	H bond acceptors	3	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	1	ACD/ALogP	0.93
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.34 g/cm ³
SMILES	O=S(=O)(O)c1ccc(cc1)C				
InChIKey	JOXIMZWYDAKGHI-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.12	0.01	2.69
ethanol	4.69	0.41	260.62
toluene	0.00	0.00	0.00

p-toluenesulfonylmethyl isocyanide C₉H₉NO₂S²⁰⁸



Compound Data					
Molecular weight	195.238	H bond acceptors	3	Rule of 5 violations	0
Compound type	isonitrile	H bond donors	0	ACD/ALogP	†
Phase 25°C	solid	Rotatable bonds	2	Predicted density	‡
SMILES	O=S(=O)(c1ccc(cc1)C)C[N+]#[C-]				
InChIKey	CFOAUYCPAUGDFF-UHFFFAOYSA-N				

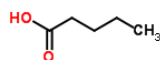
Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.88	‡	‡
chloroform	0.21	‡	‡
ethanol	0.18	‡	‡
THF	1.86	‡	‡
toluene	0.14	‡	‡

† ACD/ALogP prediction fail.

‡ Solute density prediction fail.

pentanoic acid C₅H₁₀O₂²²

Compound Data			
Molecular weight	102.132	H bond acceptors	2
		Rule of 5 violations	0

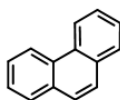


Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.31
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.966 g/cm ³
SMILES	<chem>CCCC(=O)O</chem>				
InChIKey	NQPDZGIKBWPEJ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.19	0.93	4393.39

phenanthrene C₁₄H₁₀⁹⁰²



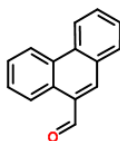
Compound Data

Molecular weight	178.229	H bond acceptors	0	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	4.68
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.13 g/cm ³
SMILES	<chem>c3cc2ccc1ccccc1c2cc3</chem>				
InChIKey	YNPNZTXNASCQKK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
benzene	2.02	0.21	60.52
carbon disulfide	3.05	0.26	83.20
carbon tetrachloride	1.73	0.18	24.99
diethyl ether	1.36	0.15	42.04
ethanol	0.21	0.01	4.96
hexane	0.32	0.04	8.90

phenanthrene-9-carboxaldehyde C₁₅H₁₀O^{30, 60, 4, 136, 242, 51, 24}



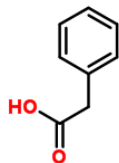
Compound Data

Molecular weight	206.239	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	4.1
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.217 g/cm ³
SMILES	<chem>O=Cc2cc3c(c1c2cccc1)ccccc3</chem>				
InChIKey	QECIGCMPORCORE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1,1,2-trichlorotrifluoroethane	0.02	0.00	0.25
2-propanol	0.07	0.01	1.85
acetonitrile	0.16	0.01	4.39
benzene	0.66	0.06	17.56
chloroform	0.04	0.00	0.55
cyclohexane	0.07	0.01	1.85
cyclopentane	0.03	0.00	0.79
dichloromethane	0.00	0.00	0.00
diethyl ether	0.1	0.01	2.86
DMF	1.25	0.12	37.60
DMSO	0.77	0.06	16.62
ethanol	0.1	0.01	2.69
hexane	0.07	0.01	2.16
methanol	0.11	0.00	2.93
THF	2.32	0.23	87.22

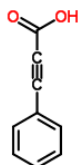
phenylacetic acid C₈H₈O₂^{86, 123}



Compound Data			
Molecular weight	136.148	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.51
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.164 g/cm ³
SMILES	O=C(O)Cc1ccccc1		
InChIKey	WLJVXDMOQOQPHL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	3.87	0.28	128.87
benzene	3.35	0.33	85.91
DMF	3.76	0.36	105.03
DMSO	6.35	0.64	305.77
THF	5.62	0.57	247.02
toluene	1.94	0.21	39.23

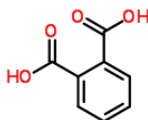
phenylpropynoic acid C₉H₆O₂^{98, 82, 85}



Compound Data			
Molecular weight	146.143	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.61
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.24 g/cm ³
SMILES	O=C(C#Cc1ccccc1)O		
InChIKey	XNERWVPQCYSMLC-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.38	0.08	32.24
DMSO	3.33	0.28	72.89
methanol	2.89	0.16	85.06
THF	4.34	0.42	143.85

phthalic acid C₈H₆O₄^{138, 47}



Compound Data			
Molecular weight	166.131	H bond acceptors	4 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.81
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.451 g/cm ³
SMILES	O=C(O)c1ccccc1C(=O)O		
InChIKey	XNGIFLGASWRNHJ-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.51	0.04	6.00
methanol	0.43	0.02	9.98

piperal C₈H₆O₃^{71, 30}

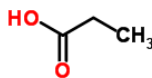
Compound Data			
Molecular weight	150.131	H bond acceptors	3 Rule of 5 violations 0

Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.05
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.337 g/cm ³
SMILES	<chem>O=Cc1ccc2OCOc2c1</chem>				
InChIKey	SATCULPHIDODRE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p _{pph} (g/100g)
acetonitrile	7.11	0.66	708.73
chloroform	7.95	0.86	741.57
dichloromethane	7.59	0.78	616.11
diethyl ether	6.38	0.69	460.15
DMSO	6.05	0.57	257.75
ethanol	4.99	0.40	218.45
hexane	0.15	0.02	3.39
methanol	7.29	0.63	798.18
THF	7.44	0.78	750.82
toluene	6.4	0.71	392.09

propanoic acid $\text{C}_3\text{H}_6\text{O}_2^{22}$

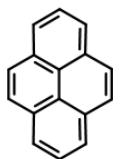


		Compound Data			
Molecular weight	74.0785	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.25
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.019 g/cm ³
SMILES	CCC(=O)O				
InChIKey	XBDOKXXYIPTUBI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p _{pph} (g/100g)
methanol	13.41	0.96	5249.72

pyrene C₁₆H₁₀^{108, 109}



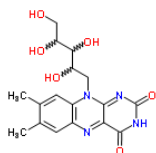
		Compound Data			
Molecular weight	202.251	H bond acceptors	0	Rule of 5 violations	1
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	5.17
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.248 g/cm ³
SMILES	c3ccc2ccc1ccccc4c1c2ccc4				
InChIKey	BBEAOIROQSPTKN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.1	0.01	2.75

riboflavin $\text{C}_{17}\text{H}_{20}\text{N}_4\text{O}_6$ ⁴⁶

		Compound Data			
Molecular weight	376.364	H bond acceptors	10	Rule of 5 violations	2
Compound type	non-Ugi related	H bond donors	5	ACD/ALogP	-2.02
Phase 25°C	solid	Rotatable bonds	9	Predicted density	1.65 g/cm ³
SMILES	O=C2/N=C1/N(c3cc(c(cc3/N=C1/C(=O)N2)C)C)CC(O)C(O)C(O)C(O)C				



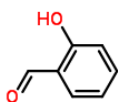
InChIKey

AUNGANRZJHBGPY-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.00	0.00	0.00

salicylaldehyde $C_7H_6O_2$ ²¹



Compound Data

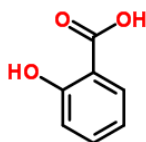
Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.61
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.226 g/cm ³
SMILES	<chem>c1cccc(C=O)c1O</chem>				
InChIKey	SMQUZDBALVYZAC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.04	□	□

□ Solute is very soluble/miscible, conversion fail.

salicylic acid $C_7H_6O_3$ ^{34, 901, 902, 138, 52}



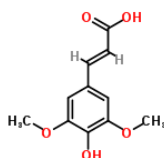
Compound Data

Molecular weight	138.121	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	2.06
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.375 g/cm ³
SMILES	<chem>O=C(O)c1ccccc1O</chem>				
InChIKey	YGSDEFSJMLZEOE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.19	0.01	1.74
dichloromethane	0.15	0.01	1.68
ethanol	2.34	0.15	54.17
methanol	2.65	0.13	66.24
toluene	0.11	0.01	1.76

sinapic acid $C_{11}H_{12}O_5$ ^{25, 2}



Compound Data

Molecular weight	224.21	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	1.29
Phase 25°C	solid	Rotatable bonds	5	Predicted density	1.307 g/cm ³
SMILES	<chem>O=C(O)/C=C/c1cc(OC)c(O)c(OC)c1</chem>				
InChIKey	PCMORTLOPMLEFB-ONEGZZNKSA-N				

Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
ethanol	0.79	0.05	26.27
methanol	1.04	0.05	37.69
THF	0.45	0.04	11.95

sodium chloride $\text{ClNa}^{1, 207, 900}$



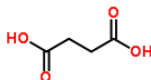
Compound Data				
Molecular weight	58.4428	H bond acceptors	0	Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP †
Phase 25°C	solid	Rotatable bonds	0	Predicted density ‡
SMILES	<chem>[Cl][Na]</chem>			
InChIKey	FAPWRFPFISZLT-UHFFFAOYSA-M			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.22	‡	‡
THF	0.04	‡	‡

† ACD/ALogP prediction fail.

‡ Solute density prediction fail.

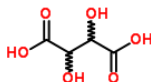
succinic acid $\text{C}_4\text{H}_6\text{O}_4^{45, 42, 44}$



Compound Data				
Molecular weight	118.088	H bond acceptors	4	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP -0.59
Phase 25°C	solid	Rotatable bonds	3	Predicted density 1.408 g/cm ³
SMILES	<chem>OC(=O)CCC(=O)O</chem>			
InChIKey	KDYFGRWQOYBRFD-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.34	0.03	5.22
ethanol	0.57	0.03	9.06

tartaric acid $\text{C}_4\text{H}_6\text{O}_6^{38}$

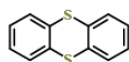


Compound Data				
Molecular weight	150.087	H bond acceptors	6	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	4	ACD/ALogP -1.43
Phase 25°C	solid	Rotatable bonds	5	Predicted density 1.886 g/cm ³
SMILES	<chem>C(C(C(=O)O)O)(C(=O)O)O</chem>			
InChIKey	FEWJPZIEWOKRBE-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	0.79	0.06	16.39

thianthrene $\text{C}_{12}\text{H}_8\text{S}_2^{905}$

Compound Data				
Molecular weight	216.322	H bond acceptors	0	Rule of 5 violations 0

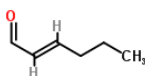


Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	4.57
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.31 g/cm ³
SMILES	<chem>S1c3c(Sc2ccccc2)cccc3</chem>				
InChIKey	GVIIJXMXTUZIOD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-decanol	0.04	0.01	1.05
1,4-dioxane	0.27	0.02	6.14
acetonitrile	0.02	0.00	0.58
decane	0.03	0.01	0.89
diethyl ether	0.08	0.01	2.39
diisopropyl ether	0.05	0.01	1.44
ethylene glycol	0.02	0.00	0.40
hexadecane	0.03	0.01	0.84
nonane	0.03	0.01	0.90
undecane	0.03	0.01	0.88

trans-2-hexen-1-al C₆H₁₀O²²



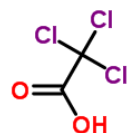
Molecular weight	98.143	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.58
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.828 g/cm ³
SMILES	<chem>CCCC=CC=O</chem>				
InChIKey	MBDOYVRWFFCFHM-SNAWJCMRSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.62	□	□

□ Solute is very soluble/miscible, conversion fail.

trichloroacetic acid C₂HCl₃O₂²²



Molecular weight	163.387	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.67
Phase 25°C	liquid	Rotatable bonds	0	Predicted density	1.807 g/cm ³
SMILES	<chem>C(=O)(C(Cl)(Cl)Cl)O</chem>				
InChIKey	YNJBWRMUSHSURL-UHFFFAOYSA-N				

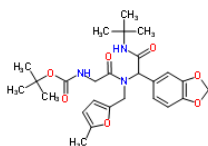
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.91	0.80	2068.61

UCExp216-3A C₂₆H₃₅N₃O₇¹¹³

Compound Data

Molecular weight	501.572	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.06

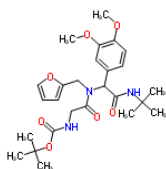


Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.209 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(c1ccc2OCOC2c1)N(Cc3ccc(C)oc3)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.73
DMSO	0.28	0.02	14.46
ethanol	0.03	0.00	1.95
methanol	0.06	0.00	4.10
toluene	0.01	0.00	0.58

Ugi product 104C (UC) C₂₆H₃₇N₃O₇⁶⁵



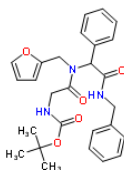
Compound Data

Molecular weight	503.588	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	3.48
Phase 25°C	solid	Rotatable bonds	12	Predicted density	1.156 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccco1)C(c2ccc(OC)c(OC)c2)C(=O)NC(C)(C)C</chem>				
InChIKey	RXLIYJRDQONCRV-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.29	0.01	22.20

Ugi product 108C (UC) C₂₇H₃₁N₃O₅⁶⁵



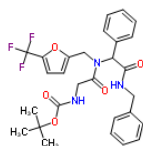
Compound Data

Molecular weight	477.552	H bond acceptors	8	Rule of 5 violations	0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.43
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.198 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccco1)C(c2ccccc2)C(=O)NCc3ccccc3</chem>				
InChIKey	COBIEQVPXUIPRH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.36	0.02	26.66

Ugi product 109C(UC) C₂₈H₃₀F₃N₃O₅⁶⁵



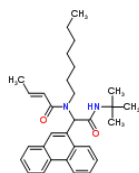
Compound Data

Molecular weight	545.55	H bond acceptors	8	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	5
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.263 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccc(o1)C(F)(F)F)C(c2ccccc2)C(=O)NCc3ccccc3</chem>				
InChIKey	XRHVBZVUCGMHPN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.15	0.01	11.62

Ugi product 148B C₃₁H₄₀N₂O₂^{96, 145}



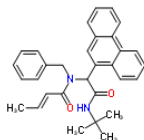
Compound Data

Molecular weight	472.661	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	7.47
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.067 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(CCCCCC)C(=O))C=C(C)c2cc3ccccc3c1ccccc12</chem>				
InChIKey	HOKCULFCASQT-FRKPEAEDSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.02	0.00	1.28
benzene	0.05	0.00	2.77
ethanol	0.00	0.00	0.00
methanol	0.03	0.00	1.91
THF	0.4	0.04	25.03
toluene	0.14	0.02	8.10

Ugi product 150D(UC) C₃₁H₃₂N₂O₂^{78, 65}



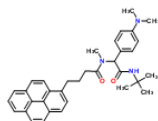
Compound Data

Molecular weight	464.598	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.18
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.148 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O))C=C(C)c3cc4ccccc4c2ccccc23</chem>				
InChIKey	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.53
DMSO	0.18	0.01	8.21
ethanol	0.04	0.00	2.42
methanol	0.07	0.00	4.12
THF	0.49	0.05	31.41
toluene	0.04	0.00	2.17

Ugi product 171K (UC) C₃₅H₃₉N₃O₂⁶⁵



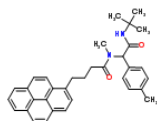
Compound Data

Molecular weight	533.703	H bond acceptors	5	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.83
Phase 25°C	solid	Rotatable bonds	9	Predicted density	1.177 g/cm ³
SMILES	<chem>CN(C)c1ccc(cc1)C(C(=O)NC(C)(C)N(C)C(=O))CCc5ccc4ccc3ccccc2ccc5c4c23</chem>				
InChIKey	XWJCEFGKUMNBLK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.02	0.00	1.43

Ugi product 173B (UC) C₃₄H₃₆N₂O₂⁶⁵

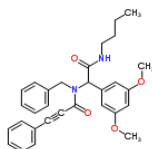


Compound Data				
Molecular weight	504.662	H bond acceptors	4	Rule of 5 violations 2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP 7.18
Phase 25°C	solid	Rotatable bonds	8	Predicted density 1.169 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(C)C(=O)CCCc4ccc3ccc2ccccc1ccc4c3c12)c5ccc(C)cc5</chem>			
InChIKey	KNHNINYGWDFMQZ-UHFFFAOYSA-N			

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.08	0.00	5.55

Ugi product 173G (UC) C₃₀H₃₂N₂O₄⁶⁵

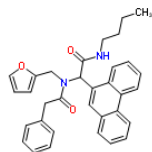


Compound Data				
Molecular weight	484.586	H bond acceptors	6	Rule of 5 violations 1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP 6.39
Phase 25°C	solid	Rotatable bonds	11	Predicted density 1.19 g/cm ³
SMILES	<chem>COc1cc(cc(OC)c1)C(C(=O)NCCCC)N(Cc2ccccc2)C(=O)C#Cc3ccccc3</chem>			
InChIKey	VOGZWAORWZGOTE-UHFFFAOYSA-N			

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.18	0.01	12.50

Ugi product 176C (UC) C₃₃H₃₂N₂O₃^{127, 145, 65}



Compound Data				
Molecular weight	504.619	H bond acceptors	5	Rule of 5 violations 2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP 6.9
Phase 25°C	solid	Rotatable bonds	10	Predicted density 1.197 g/cm ³
SMILES	<chem>O=C(Cc1ccccc1)N(Cc2ccco2)C(c4cc5ccccc5c3ccccc34)C(=O)NCCCC</chem>			
InChIKey	RGGYLRDGJAJCY-UHFFFAOYSA-N			

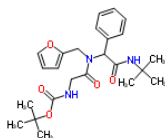
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1,4-dioxane	0.19	0.02	10.47
acetonitrile	0.02	0.00	1.36
benzene	0.03	0.00	1.76
diethyl ether	0.02	0.00	1.39
DMF	0.27	0.02	17.67
DMSO	0.19	0.01	9.48
ethanol	0.01	0.00	0.65
methanol	0.05	0.00	3.42
THF	0.28	0.02	17.72
toluene	0.03	0.00	1.76

Ugi product 206B(UC) C₂₄H₃₃N₃O₅⁵⁶

Compound Data

Molecular weight	443.536	H bond acceptors	8	Rule of 5 violations 0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP 3.74
Phase 25°C	solid	Rotatable bonds	10	Predicted density 1.145 g/cm ³



SMILES

O=C(CNC(=O)OC(C)(C)C)N(Cc1ccco1)C(c2ccccc2)C(=O)NC(C)(C)C

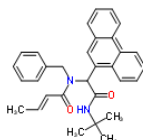
InChIKey

BXAOUWIVXLQYOZ-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.00	0.00	0.00
acetonitrile	0.02	0.00	1.20
benzene	0.01	0.00	0.51
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.57	0.06	21.63
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.24	0.02	9.37
diethyl ether	0.00	0.00	0.00
DMF	0.24	0.02	13.49
DMSO	0.23	0.02	10.19
ethanol	0.02	0.00	1.15
hexane	0.00	0.00	0.00
methanol	0.05	0.00	3.00
THF	0.26	0.02	14.19
toluene	0.01	0.00	0.51

Ugi product 214C(UC) C₃₁H₃₂N₂O₂²⁷



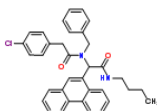
Compound Data

Molecular weight	464.598	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.18
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.148 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O)/C=C\C)c3cc4ccccc4c2ccccc23</chem>				
InChIKey	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.01	0.00	0.62
THF	0.35	0.03	20.96

Ugi product 215F(UC) C₃₅H₃₃ClN₂O₂⁷¹



Compound Data

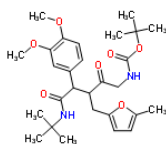
Molecular weight	549.102	H bond acceptors	4	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	8.33
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.219 g/cm ³
SMILES	<chem>Clc5ccc(CC(=O)N(Cc1ccccc1)C(c3cc4ccccc4c2ccccc23)C(=O)NCCCC)cc5</chem>				
InChIKey	NCOSMKWGNJCPCR-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.99
DMSO	0.38	0.03	22.91
ethanol	0.06	0.00	4.34
methanol	0.12	0.01	9.25

THF	0.61	0.06	51.09
toluene	0.07	0.01	4.56

Ugi Product 216-4A C₂₈H₄₀N₂O₇^{93, 97}

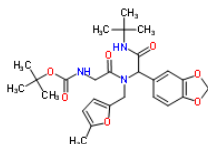


Molecular weight	516.626	H bond acceptors	9	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.08
Phase 25°C	solid	Rotatable bonds	13	Predicted density	1.12 g/cm ³
SMILES	<chem>Cc1ccc(o1)CC(C(c2ccc(c(c2)OC)OC)C(=O)NC(C)(C)C)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey					

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.13	0.01	9.17
DMSO	0.06	0.00	2.90
ethanol	0.07	0.00	4.79
methanol	0.18	0.01	13.47
toluene	0.2	0.02	13.07

Ugi product 62E (UC) C₂₆H₃₅N₃O₇⁶⁵

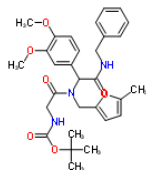


Molecular weight	501.572	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.06
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.209 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(c1ccc2OCOc2c1)N(Cc3ccc(C)o3)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.13	0.01	9.15

Ugi product 64C (UC) C₃₀H₃₇N₃O₇⁶⁵



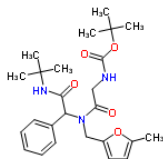
Molecular weight	551.631	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.63
Phase 25°C	solid	Rotatable bonds	13	Predicted density	1.192 g/cm ³
SMILES	<chem>CC(C)(C)OC(=O)NCC(=O)N(Cc1ccc(C)o1)C(C(=O)NCc2cccc2)c3ccc(OC)c(OC)c3</chem>				
InChIKey	VMMFSZQZVZNXSXSK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.03	0.00	2.23

Ugi product 86B (UC) C₂₅H₃₅N₃O₅⁶⁵

Compound Data

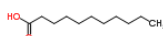


Molecular weight	457.562	H bond acceptors	8	Rule of 5 violations	0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.2
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.133 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccc(C)cc1)C(c2ccccc2)C(=O)NC(C)(C)C</chem>				
InChIKey	WDAGUORBKBNETC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.17	0.01	11.09

undecanoic acid C₁₁H₂₂O₂⁵⁸

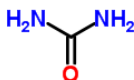


Molecular weight	186.291	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	4.5
Phase 25°C	solid	Rotatable bonds	9	Predicted density	0.909 g/cm ³
SMILES	<chem>O=C(O)CCCCCCCCC</chem>				
InChIKey	ZDPHROEEEOARMN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.94	0.55	488.75
methanol	4	0.49	549.05

urea CH₄N₂O⁵³

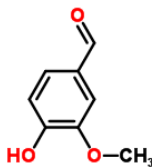


Molecular weight	60.0553	H bond acceptors	3	Rule of 5 violations	0
Compound type	amide	H bond donors	4	ACD/ALogP	-2.11
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.212 g/cm ³
SMILES	<chem>NC(=O)N</chem>				
InChIKey	XSQUKJJFZCRTK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	2.66	0.12	24.44

vanillin C₈H₈O₃^{906, 4, 10, 11, 55, 207, 19}



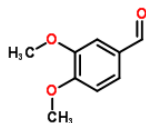
Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm ³
SMILES	<chem>Oc1ccc(cc1OC)C=O</chem>				
InChIKey	MWOOGOJBHIARFG-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	1.82	0.15	44.94
1,2-dichloroethane	1.17	0.10	17.74
acetonitrile	2.36	0.15	67.86
butanone	2.14	0.21	56.32

ethanol	2.47	0.17	69.35
methanol	4.16	0.27	173.01
THF	3.6	0.34	108.89
toluene	0.3	0.03	5.44

veratraldehyde C₉H₁₀O₃^{41, 71, 208}



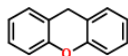
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.61
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.114 g/cm ³
SMILES	COc1cc(ccc1OC)C=O				
InChIKey	WJUFSDZVCOTFON-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	3.03	0.29	119.01
acetonitrile	5.76	0.69	904.54
chloroform	5.7	0.75	421.71
dichloromethane	6.06	0.81	837.51
diethyl ether	3.55	0.43	170.84
DMSO	5.31	0.64	386.17
ethanol	5.49	0.64	645.97
hexane	0.07	0.01	1.74
methanol	5.87	0.67	1041.50
THF	5.34	0.68	480.29
toluene	4.54	0.60	267.44

xanthene C₁₃H₁₀O⁹⁰⁵



Compound Data

Molecular weight	182.218	H bond acceptors	1	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	3.93
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.159 g/cm ³
SMILES	O2c1ccccc1Cc3c2ccccc3				
InChIKey	GJCOSYZMQJWQCA-UHFFFAOYSA-N				

Solubility Data

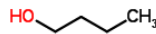
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.19	0.02	4.43
1-decanol	0.24	0.05	5.49
1-heptanol	0.23	0.03	5.30
1-hexanol	0.22	0.03	5.09
1-octanol	0.24	0.04	5.52
1-pentanol	0.2	0.02	4.64
1-propanol	0.15	0.01	3.52
1,2-dichloroethane	1.62	0.15	33.77
2-butanol	0.13	0.01	3.02
2-methyl-1-pentanol	0.16	0.02	3.67
2-methyl-1-propanol	0.12	0.01	2.78
2-methyl-2-butanol	0.18	0.02	4.16
2-methyl-2-propanol	0.12	0.01	2.77
2-pentanol	0.16	0.02	3.70
2-propanol	0.11	0.01	2.58
2,2,4-trimethylpentane	0.15	0.02	3.95
3-methyl-1-butanol	0.15	0.02	3.46
4-methyl-2-pentanol	0.14	0.02	3.22

acetonitrile	0.35	0.02	9.03
carbon tetrachloride	1.25	0.12	16.71
cyclohexane	0.39	0.04	9.58
cyclooctane	0.38	0.05	9.32
cyclopentanol	0.33	0.03	6.32
decane	0.24	0.05	6.19
dibutyl ether	0.5	0.08	12.68
diethyl ether	0.79	0.08	22.39
diisopropyl ether	0.41	0.06	10.54
ethanol	0.1	0.01	2.37
heptane	0.24	0.03	6.54
hexadecane	0.24	0.07	5.88
hexane	0.23	0.03	6.44
methanol	0.1	0.00	2.46
methyl tert-butyl ether	0.65	0.08	17.59
methylcyclohexane	0.33	0.04	8.17
nonane	0.24	0.04	6.28
octane	0.25	0.04	6.67
undecane	0.23	0.05	5.85

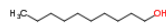
Solvents

Below we present data for the solvents used in the Open Notebook Science Challenge. We present various properties such as density and boiling point together with important solvation related parameters such as dielectric constants and dipole moments [1000-1100].

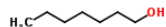
1-butanol

	Compound Data
	Molecular weight 74.1216
	Predicted density 0.805 g/cm ³
	Boiling point 117.7 °C
	Dipole moment 1.66
	Dielectric constant 17.8
	SMILES CCCC
	InChIKey LRHPLDGYMQRHN-UHFFFAOYSA-N

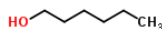
1-decanol

	Compound Data
	Molecular weight 158.2811
	Predicted density 0.828 g/cm ³
	Boiling point 227.8 °C
	SMILES OCCCCCCCCC
	InChIKey MWKFXSUHUHTGQN-UHFFFAOYSA-N

1-heptanol

	Compound Data
	Molecular weight 116.2013
	Predicted density 0.82 g/cm ³
	Boiling point 176.9 °C
	SMILES OCCCCCC
	InChIKey BBMCTIGTCKYKF-UHFFFAOYSA-N

1-hexanol



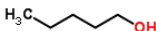
Compound Data	
Molecular weight	102.1748
Predicted density	0.816 g/cm ³
Boiling point	158.2 °C
Dipole moment	1.55
Dielectric constant	13.3
SMILES	OCCCCC
InChIKey	ZSIAUFGUXNUGDI-UHFFFAOYSA-N

1-octanol



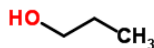
Compound Data	
Molecular weight	130.2279
Predicted density	0.823 g/cm ³
Boiling point	194.7 °C
SMILES	CCCCCCCC
InChIKey	KBPLFHHGFOOTCA-UHFFFAOYSA-N

1-pentanol



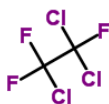
Compound Data	
Molecular weight	88.1482
Predicted density	0.811 g/cm ³
Boiling point	138.5 °C
SMILES	CCCCC
InChIKey	AMQJEAYHLZJPGS-UHFFFAOYSA-N

1-propanol



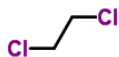
Compound Data	
Molecular weight	60.095
Predicted density	0.795 g/cm ³
Boiling point	95.8 °C
Dipole moment	1.68
Dielectric constant	20.1
SMILES	CCCO
InChIKey	BDERNNFJNOPAEC-UHFFFAOYSA-N

1,1,2-trichlorotrifluoroethane



Compound Data	
Molecular weight	187.3756
Predicted density	1.67 g/cm ³
Boiling point	50.9 °C
SMILES	ClC(F)(F)C(Cl)(Cl)F
InChIKey	AJDIZQLSFPQPEY-UHFFFAOYSA-N

1,2-dichloroethane



Compound Data

Molecular weight	98.9592
Predicted density	1.173 g/cm ³
Boiling point	83.5 °C
SMILES	ClCCCl
InChIKey	WSLDOOZREJYCGB-UHFFFAOYSA-N

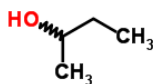
1,4-dioxane



Compound Data

Molecular weight	88.1051
Predicted density	0.995 g/cm ³
Boiling point	102.9 °C
SMILES	O1CCOCC1
InChIKey	RYHBNJHYFVUHQT-UHFFFAOYSA-N

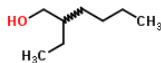
2-butanol



Compound Data

Molecular weight	74.1216
Predicted density	0.801 g/cm ³
Boiling point	96.6 °C
SMILES	OC(C)CC
InChIKey	BTANRVKQNVYAZ-UHFFFAOYSA-N

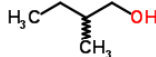
2-ethyl-1-hexanol



Compound Data

Molecular weight	130.2279
Predicted density	0.821 g/cm ³
Boiling point	184.6 °C
SMILES	OCC(CC)CCCC
InChIKey	YIWUKEYIRIRTPP-UHFFFAOYSA-N

2-methyl-1-butanol



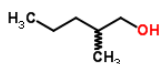
Compound Data

Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	128.7 °C
SMILES	OCC(C)CC
InChIKey	QPRQEDXDYOZYLA-UHFFFAOYSA-N

2-methyl-1-pentanol

Compound Data

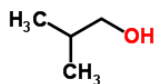
Molecular weight	102.1748
Predicted density	0.814 g/cm ³



Boiling point	148 °C
SMILES	<chem>OCC(C)CC</chem>
InChIKey	PFNHSEQQEPMLNI-UHFFFAOYSA-N

2-methyl-1-propanol

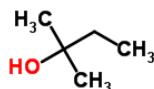
Compound Data



Molecular weight	74.1216
Predicted density	0.801 g/cm ³
Boiling point	105 °C
SMILES	<chem>OCC(C)C</chem>
InChIKey	ZXEKIHBDNHEJCQ-UHFFFAOYSA-N

2-methyl-2-butanol

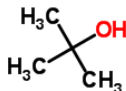
Compound Data



Molecular weight	88.1482
Predicted density	0.811 g/cm ³
Boiling point	102 °C
SMILES	<chem>OC(C)(C)CC</chem>
InChIKey	MSXVEPNJUHWQHW-UHFFFAOYSA-N

2-methyl-2-propanol

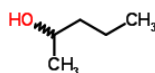
Compound Data



Molecular weight	74.1216
Predicted density	0.804 g/cm ³
Boiling point	84.6 °C
SMILES	<chem>OC(C)(C)C</chem>
InChIKey	DKGAVHZHDRPRBM-UHFFFAOYSA-N

2-pentanol

Compound Data

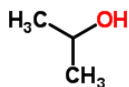


Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	118.8 °C
SMILES	<chem>OC(C)CCC</chem>
InChIKey	JYVLIDXNZAXMDK-UHFFFAOYSA-N

2-propanol

Compound Data

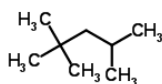
Molecular weight	60.095
Predicted density	0.791 g/cm ³
Boiling point	73 °C



Dipole moment	1.66
Dielectric constant	1.89
SMILES	CC(O)C
InChIKey	KFZMGEQAYNKOFK-UHFFFAOYSA-N

2,2,4-trimethylpentane

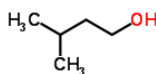
Compound Data



Molecular weight	114.2285
Predicted density	0.709 g/cm ³
Boiling point	98.8 °C
SMILES	CC(C)CC(C)(C)C
InChIKey	NHTMVDHEPJAVLT-UHFFFAOYSA-N

3-methyl-1-butanol

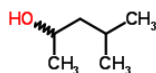
Compound Data



Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	131.2 °C
SMILES	OCCCC(C)C
InChIKey	PHTQWCKDNZKARW-UHFFFAOYSA-N

4-methyl-2-pentanol

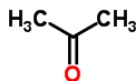
Compound Data



Molecular weight	102.1748
Predicted density	0.811 g/cm ³
Boiling point	133.5 °C
SMILES	OC(C)CC(C)C
InChIKey	WVYWICLMDOOCFB-UHFFFAOYSA-N

acetone

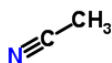
Compound Data



Molecular weight	58.0791
Predicted density	0.772 g/cm ³
Boiling point	46.5 °C
Dipole moment	2.88
Dielectric constant	20.7
SMILES	CC(=O)C
InChIKey	CSCPPACGZOO CGX-UHFFFAOYSA-N

acetonitrile

Compound Data



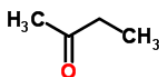
Molecular weight	41.0519
Predicted density	0.747 g/cm ³
Boiling point	63.5 °C
Dipole moment	3.92
Dielectric constant	36.6
SMILES	CCN
InChIKey	QUSNBJAOOMFDIB-UHFFFAOYSA-N

benzene



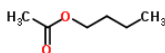
Compound Data	
Molecular weight	78.1118
Predicted density	0.873 g/cm ³
Boiling point	78.8 °C
Dipole moment	0
Dielectric constant	2.28
SMILES	c1ccccc1
InChIKey	UHOVQNZJYSORNB-UHFFFAOYSA-N

butanone



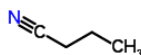
Compound Data	
Molecular weight	72.1057
Predicted density	0.786 g/cm ³
Boiling point	75.6 °C
SMILES	CC(=O)CC
InChIKey	ZWEHNKRNPVVGH-UHFFFAOYSA-N

butyl acetate



Compound Data	
Molecular weight	116.1583
Predicted density	0.886 g/cm ³
Boiling point	126.6 °C
SMILES	CC(=O)OCCCC
InChIKey	DKPFZGUDAPQIHT-UHFFFAOYSA-N

butyronitrile



Compound Data	
Molecular weight	69.1051
Predicted density	0.785 g/cm ³
Boiling point	117.3 °C
SMILES	N#CCCC
InChIKey	KVNRLNFWIYMESJ-UHFFFAOYSA-N

carbon disulfide

Compound Data



Molecular weight	76.1407
Predicted density	1.259 g/cm ³
Boiling point	46.2 °C
SMILES	S=C=S
InChIKey	QGJOPFRUJISHPQ-UHFFFAOYSA-N

carbon tetrachloride



Compound Data	
Molecular weight	153.8227
Predicted density	1.697 g/cm ³
Boiling point	76 °C
Dipole moment	0
Dielectric constant	2.24
SMILES	[C](Cl)(Cl)(Cl)Cl
InChIKey	VZGDMQKNWNREIO-UHFFFAOYSA-N

chloroform



Compound Data	
Molecular weight	119.3776
Predicted density	1.5 g/cm ³
Boiling point	61.2 °C
Dipole moment	1.15
Dielectric constant	5.5
SMILES	C(Cl)(Cl)Cl
InChIKey	HEDRZPFGACZZDS-UHFFFAOYSA-N

cyclohexane



Compound Data	
Molecular weight	84.1595
Predicted density	0.79 g/cm ³
Boiling point	80.7 °C
Dipole moment	0
Dielectric constant	18.5
SMILES	C1CCCCC1
InChIKey	XDTMQSROBMDMFD-UHFFFAOYSA-N

cyclooctane



Compound Data	
Molecular weight	112.2126
Predicted density	0.79 g/cm ³
Boiling point	152 °C
SMILES	C1CCCCCCC1
InChIKey	WJTCGQSWYFHTAC-UHFFFAOYSA-N

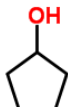
cyclopentane



Compound Data

Molecular weight	70.1329
Predicted density	0.79 g/cm ³
Boiling point	49.2 °C
SMILES	C1CCCC1
InChIKey	RGSFGYAAUTVSQA-UHFFFAOYSA-N

cyclopentanol



Compound Data

Molecular weight	86.1323
Predicted density	1.004 g/cm ³
Boiling point	140.8 °C
SMILES	OC1CCCC1
InChIKey	XCIXKGXIYUWCLL-UHFFFAOYSA-N

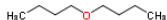
decane



Compound Data

Molecular weight	142.2817
Predicted density	0.734 g/cm ³
Boiling point	174.9 °C
SMILES	C(CCCCCCCC)C
InChIKey	DIOQZVSQGTUSAI-UHFFFAOYSA-N

dibutyl ether



Compound Data

Molecular weight	130.2279
Predicted density	0.78 g/cm ³
Boiling point	142.1 °C
SMILES	O(CCCC)CCCC
InChIKey	DURPTKYDGMDSBL-UHFFFAOYSA-N

dichloromethane

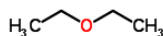


Compound Data

Molecular weight	84.9326
Predicted density	1.252 g/cm ³
Boiling point	39.6 °C
Dipole moment	1.6
Dielectric constant	9.08
SMILES	C(Cl)Cl
InChIKey	YMWUJEATGCHHMB-UHFFFAOYSA-N

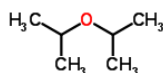
diethyl ether

Compound Data



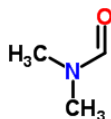
Molecular weight	74.1216
Predicted density	0.734 g/cm ³
Boiling point	33.2 °C
Dipole moment	1.15
Dielectric constant	4.34
SMILES	CCOCC
InChIKey	RTZKZFJDLAIYFH-UHFFFAOYSA-N

diisopropyl ether



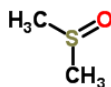
Compound Data	
Molecular weight	102.1748
Predicted density	0.758 g/cm ³
Boiling point	68.3 °C
SMILES	O(C(C)C)C(C)C
InChIKey	ZAFNJMIOETHYRJ-UHFFFAOYSA-N

DMF



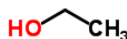
Compound Data	
Molecular weight	73.0938
Predicted density	0.87 g/cm ³
Boiling point	153 °C
Dipole moment	3.82
Dielectric constant	38.3
SMILES	O=C(NC)C
InChIKey	OHLUHNLEMFGTQ-UHFFFAOYSA-N

DMSO



Compound Data	
Molecular weight	78.1334
Predicted density	1.099 g/cm ³
Boiling point	189 °C
Dipole moment	3.96
Dielectric constant	47.2
SMILES	CS(=O)C
InChIKey	IAZDPXIOMUYVGZ-UHFFFAOYSA-N

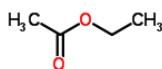
ethanol



Compound Data	
Molecular weight	46.0684
Predicted density	0.78 g/cm ³
Boiling point	72.6 °C
Dipole moment	1.69
Dielectric constant	24.3
SMILES	CCO

InChIKey LFQSCWFLJHTTHZ-UHFFFAOYSA-N

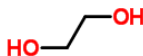
ethyl acetate



Compound Data

Molecular weight	88.1051
Predicted density	0.898 g/cm ³
Boiling point	73.9 °C
Dipole moment	1.78
Dielectric constant	6.02
SMILES	CCOC(=O)C1=NN(C(=N1)C(C1)(Cl)Cl)C2=C(C=C(C=C2)Cl)Cl
InChIKey	GMBRUAIJEFRHFQ-UHFFFAOYSA-N

ethylene glycol



Compound Data

Molecular weight	62.0678
Predicted density	1.097 g/cm ³
Boiling point	197.5 °C
SMILES	OCCO
InChIKey	LYCAIKOWRPUZTN-UHFFFAOYSA-N

heptane



Compound Data

Molecular weight	100.2019
Predicted density	0.695 g/cm ³
Boiling point	98.8 °C
SMILES	CCCCCCC
InChIKey	IMNFDUFMRHMDMM-UHFFFAOYSA-N

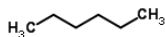
hexadecane



Compound Data

Molecular weight	226.4412
Predicted density	0.773 g/cm ³
Boiling point	286.6 °C
SMILES	CCCCCCCCCCCCCCCC
InChIKey	DCAYPVUWAIABOU-UHFFFAOYSA-N

hexane



Compound Data

Molecular weight	86.1754
Predicted density	0.675 g/cm ³
Boiling point	68.5 °C
Dipole moment	0.08
Dielectric constant	2.02
SMILES	CCCCCC
InChIKey	VLKZOEYAKHREP-UHFFFAOYSA-N

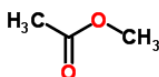
methanol



Compound Data

Molecular weight	32.0419
Predicted density	0.753 g/cm ³
Boiling point	48.1 °C
Dipole moment	1.7
Dielectric constant	33
SMILES	CO
InChIKey	OKKJLVBELUTLKV-UHFFFAOYSA-N

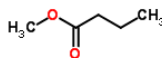
methyl acetate



Compound Data

Molecular weight	74.0785
Predicted density	0.908 g/cm ³
Boiling point	44 °C
SMILES	CC(=O)OC
InChIKey	KKKVLQRXCPHEJC-UHFFFAOYSA-N

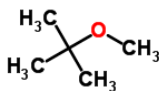
methyl butyrate



Compound Data

Molecular weight	102.1317
Predicted density	0.891 g/cm ³
Boiling point	104.2 °C
SMILES	CCCC(=O)OC
InChIKey	UUIQMZJEGPQKFD-UHFFFAOYSA-N

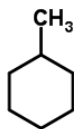
methyl tert-butyl ether



Compound Data

Molecular weight	88.1482
Predicted density	0.75 g/cm ³
Boiling point	55.2 °C
SMILES	CC(C)(C)OC
InChIKey	BZLVMXJERCGZMT-UHFFFAOYSA-N

methylcyclohexane

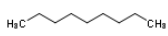


Compound Data

Molecular weight	98.1861
Predicted density	0.776 g/cm ³
Boiling point	101.1 °C
SMILES	CC1CCCCC1
InChIKey	UAEPNZWRGJTJPN-UHFFFAOYSA-N

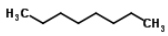
nonane

Compound Data

	Molecular weight	128.2551
	Predicted density	0.724 g/cm ³
	Boiling point	151.7 °C
	SMILES	CCCCCCCC
	InChIKey	BKIMMITUMNQMOS-UHFFFAOYSA-N

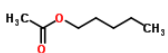
octane

Compound Data

	Molecular weight	114.2285
	Predicted density	0.711 g/cm ³
	Boiling point	126.4 °C
	SMILES	CCCCCCCC
	InChIKey	

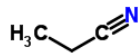
pentyl acetate

Compound Data

	Molecular weight	130.1849
	Predicted density	0.882 g/cm ³
	Boiling point	149.9 °C
	SMILES	CC(=O)OCCCC
	InChIKey	PGMYKACGEOXYJE-UHFFFAOYSA-N

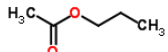
propionitrile

Compound Data

	Molecular weight	55.0785
	Predicted density	0.771 g/cm ³
	Boiling point	91.3 °C
	SMILES	N#CCC
	InChIKey	FVSKHRXBFJPNKK-UHFFFAOYSA-N

propyl acetate

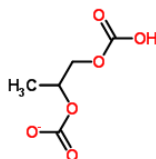
Compound Data

	Molecular weight	102.1317
	Predicted density	0.891 g/cm ³
	Boiling point	101.4 °C
	SMILES	CC(=O)OCCC
	InChIKey	YKYONYBAUNKHLG-UHFFFAOYSA-N

propylene carbonate

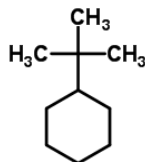
Compound Data

Molecular weight	163.106
Predicted density	1.205 g/cm ³
Boiling point	332.3 °C



SMILES OC(=O)OCC(C)OC(=O)[O-]
InChIKey ZEBXBLIKXVICMJ-UHFFFAOYSA-M

tert-butylcyclohexane



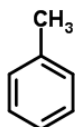
Compound Data
Molecular weight 140.2658
Predicted density 0.812 g/cm³
Boiling point 168.3 °C
SMILES CC(C)(C)C1CCCCC1
InChIKey XTVMZZBLCLWBPM-UHFFFAOYSA-N

THF



Compound Data
Molecular weight 72.1057
Predicted density 0.904 g/cm³
Boiling point 68.3 °C
Dipole moment 1.63
Dielectric constant 7.52
SMILES C1CCOC1
InChIKey WYURNTSHIVDZCO-UHFFFAOYSA-N

toluene



Compound Data
Molecular weight 92.1384
Predicted density 0.871 g/cm³
Boiling point 110.6 °C
Dipole moment 0.36
Dielectric constant 2.38
SMILES c1ccccc1C
InChIKey YXFVVABEGXRONW-UHFFFAOYSA-N

undecane



Compound Data
Molecular weight 156.3083
Predicted density 0.743 g/cm³
Boiling point 196.3 °C
SMILES C(CCCCCCCC)CC
InChIKey RSJKGSCJYTIGS-UHFFFAOYSA-N

water

Compound Data
70



Molecular weight	18.0153
Predicted density	0.998 g/cm ³
Boiling point	100 °C
SMILES	O
InChIKey	XLIFYNOQVPJJNP-UHFFFAOYSA-N

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