Appendix C

Chemical Mixing Supplemental Tables and Information

Appendix C. Chemical Mixing Supplemental Tables and Information

C.1. Supplemental Tables and Information

Table C-1. Chemicals reported to FracFocus in 10% or more of disclosures for gas-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.

Chemicals ranked by frequency of occurrence (U.S. EPA, 2015c).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Hydrochloric acid	7647-01-0	12,351	72.8%	15%
Methanol	67-56-1	12,269	72.3%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	11,897	70.1%	30%
Isopropanol	67-63-0	8,008	47.2%	30%
Water	7732-18-5	7,998	47.1%	63%
Ethanol	64-17-5	6,325	37.3%	5%
Propargyl alcohol	107-19-7	5,811	34.2%	10%
Glutaraldehyde	111-30-8	5,635	33.2%	30%
Ethylene glycol	107-21-1	5,493	32.4%	35%
Citric acid	77-92-9	4,832	28.5%	60%
Sodium hydroxide	1310-73-2	4,656	27.4%	5%
Peroxydisulfuric acid, diammonium salt	7727-54-0	4,618	27.2%	100%
Quartz	14808-60-7	3,758	22.1%	10%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	3,668	21.6%	100%
Sodium chloride	7647-14-5	3,608	21.3%	30%
Guar gum	9000-30-0	3,586	21.1%	60%
Acetic acid	64-19-7	3,563	21.0%	50%
2-Butoxyethanol	111-76-2	3,325	19.6%	10%
Naphthalene	91-20-3	3,294	19.4%	5%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,287	19.4%	30%
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	3,259	19.2%	7%
Potassium hydroxide	1310-58-3	2,843	16.8%	15%
Ammonium chloride	12125-02-9	2,483	14.6%	10%
Choline chloride	67-48-1	2,477	14.6%	75%

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	2,455	14.5%	5%
Sodium chlorite	7758-19-2	2,372	14.0%	10%
1,2,4-Trimethylbenzene	95-63-6	2,229	13.1%	1%
Carbonic acid, dipotassium salt	584-08-7	2,154	12.7%	60%
Methenamine	100-97-0	2,134	12.6%	1%
Formic acid	64-18-6	2,118	12.5%	60%
Didecyl dimethyl ammonium chloride	7173-51-5	2,063	12.2%	10%
N,N-Dimethylformamide	68-12-2	1,892	11.2%	13%
Phenolic resin	9003-35-4	1,852	10.9%	5%
Thiourea polymer	68527-49-1	1,702	10.0%	30%
Polyethylene glycol	25322-68-3	1,696	10.0%	60%

Note: Analysis considered 17,035 disclosures and 291,363 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (1,587) or other, query-specific criteria were excluded from analysis.

Table C-2. Chemicals reported to FracFocus in 10% or more of disclosures for oil-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.

Chemicals ranked by frequency of occurrence (U.S. EPA, 2015c).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Methanol	67-56-1	12,484	71.8%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	10,566	60.8%	40%
Peroxydisulfuric acid, diammonium salt	7727-54-0	10,350	59.6%	100%
Ethylene glycol	107-21-1	10,307	59.3%	30%
Hydrochloric acid	7647-01-0	10,029	57.7%	15%
Guar gum	9000-30-0	9,110	52.4%	50%
Sodium hydroxide	1310-73-2	8,609	49.5%	10%
Quartz	14808-60-7	8,577	49.4%	2%
Water	7732-18-5	8,538	49.1%	67%
Isopropanol	67-63-0	8,031	46.2%	15%
Potassium hydroxide	1310-58-3	7,206	41.5%	15%
Glutaraldehyde	111-30-8	5,927	34.1%	15%
Propargyl alcohol	107-19-7	5,599	32.2%	5%
Acetic acid	64-19-7	4,623	26.6%	30%
2-Butoxyethanol	111-76-2	4,022	23.1%	10%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,821	22.0%	5%
Sodium chloride	7647-14-5	3,692	21.2%	25%
Ethanol	64-17-5	3,536	20.3%	45%
Citric acid	77-92-9	3,310	19.0%	60%
Phenolic resin	9003-35-4	3,109	17.9%	5%
Naphthalene	91-20-3	3,060	17.6%	5%
Nonyl phenol ethoxylate	9016-45-9	2,829	16.3%	20%
Diatomaceous earth, calcined	91053-39-3	2,655	15.3%	100%
Methenamine	100-97-0	2,559	14.7%	1%
Tetramethylammonium chloride	75-57-0	2,428	14.0%	1%
Carbonic acid, dipotassium salt	584-08-7	2,402	13.8%	60%
Ethoxylated propoxylated C12-14 alcohols	68439-51-0	2,342	13.5%	2%
Choline chloride	67-48-1	2,264	13.0%	75%
Boron sodium oxide	1330-43-4	2,228	12.8%	30%
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	2,130	12.3%	50%
1,2,4-Trimethylbenzene	95-63-6	2,118	12.2%	1%

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Boric acid	10043-35-3	2,070	11.9%	25%
Polyethylene glycol	25322-68-3	2,025	11.7%	5%
2-Mercaptoethanol	60-24-2	2,012	11.6%	100%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,988	11.4%	98%
Formic acid	64-18-6	1,948	11.2%	60%
Sodium persulfate	7775-27-1	1,914	11.0%	100%
Phosphonic acid	13598-36-2	1,865	10.7%	1%
Sodium tetraborate decahydrate	1303-96-4	1,862	10.7%	30%
Potassium metaborate	13709-94-9	1,682	9.7%	60%
Ethylenediaminetetraacetic acid tetrasodium salt hydrate	64-02-8	1,676	9.6%	0%
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	1,668	9.6%	5%

Note: Analysis considered 17,640 disclosures and 385,013 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (2,268) or other, query-specific criteria were excluded from analysis.

Table C-3a. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, Alabama to Montana (U.S. EPA, 2015c).

Source: (U.S. EPA, 2015c). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Methanol	67-56-1	55 (100%)		1333 (99.7%)	228 (39.0%)	2883 (63.3%)	77 (79.4%)	596 (59.2%)	13 (92.9%)	3 (75%)	121 (62.7%)
Distillates, petroleum, hydrotreated light	64742-47-8		9 (45%)	743 (55.6%)	322 (55.0%)	3358 (73.7%)	87 (89.7%)	844 (83.9%)	14 (100%)	4 (100%)	115 (59.6%)
Ethylene glycol	107-21-1	55 (100%)	20 (100%)	291 (21.8%)	350 (59.8%)		61 (62.9%)	341 (33.9%)	10 (71.4%)	3 (75%)	95 (49.2%)
Isopropanol	67-63-0	55 (100%)	13 (65%)	586 (43.9%)		2586 (56.8%)	24 (24.7%)	515 (51.2%)	11 (78.6%)		123 (63.7%)
Quartz	14808-60-7		20 (100%)		519 (88.7%)	1048 (23.0%)	22 (22.7%)	377 (37.5%)		2 (50%)	124 (64.2%)
Sodium hydroxide	1310-73-2		20 (100%)	285 (21.3%)	403 (68.9%)	996 (21.9%)	27 (27.8%)	535 (53.2%)		2 (50%)	105 (54.4%)
Ethanol	64-17-5			603 (45.1%)		2258 (49.6%)	78 (80.4%)	420 (41.7%)		4 (100%)	
Guar gum	9000-30-0		10 (50%)		545 (93.2%)			494 (49.1%)		2 (50%)	83 (43.0%)
Hydrochloric acid	7647-01-0	55 (100%)		1330 (99.5%)		2408 (52.9%)	82 (84.5%)	569 (56.6%)			45 (23.3%)
Peroxydisulfuric acid, diammonium salt	7727-54-0		10 (50%)		484 (82.7%)		21 (21.6%)	273 (27.2%)	8 (57.1%)		119 (61.7%)

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Propargyl alcohol	107-19-7			813 (60.8%)			69 (71.1%)	299 (29.7%)	5 (35.7%)		
Glutaraldehyde	111-30-8			737 (55.1%)			73 (75.3%)	364 (36.3%)		2 (50%)	
Naphthalene	91-20-3	55 (100%)				1363 (29.9%)	41 (42.3%)	293 (29.2%)	12 (85.7%)		95 (49.2%)
2-Butoxyethanol	111-76-2	55 (100%)	20 (100%)						11 (78.6%)		
Citric acid	77-92-9						45 (46.4%)				
Saline	7647-14-5					1574 (34.5%)		408 (40.6%)		2 (50%)	
Solvent naphtha, petroleum, heavy arom.	64742-94-5					1507 (33.1%)	42 (43.3%)				135 (70.0%)
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1			375 (28.0%)			52 (53.6%)			2 (50%)	
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	55 (100%)				2215 (48.6%)			10 (71.4%)		70 (36.3%)
Potassium hydroxide	1310-58-3							340 (33.8%)		4 (100%)	115 (59.6%)
Choline chloride	67-48-1					1235 (27.1%)					
Polyethylene glycol	25322-68-3	55 (100%)							7 (50%)		69 (35.8%)
1,2,4-Trimethylbenzene	95-63-6					1211 (26.63%)	39 (40.2%)				

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Ammonium chloride	12125-02-9			277 (20.7%)		1280 (28.0%)					
Diatomaceous earth, calcined	91053-39-3		20 (100%)		417 (71.3%)						
Didecyl dimethyl ammonium chloride	7173-51-5			317 (23.7%)						2 (50%)	
Sodium chlorite	7758-19-2							352 (35.0%)		4 (100%)	
Sodium erythorbate	6381-77-7			435 (32.5%)			29 (29.9%)				
N,N-Dimethylformamide	68-12-2										
Nonyl phenol ethoxylate	9016-45-9										
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0				1150 (25.2%)	39 (40.2%)					
Sodium persulfate	7775-27-1									4 (100%)	
Tetramethylammonium chloride	75-57-0										85 (44.0%)
1,2-Propylene glycol	57-55-6								10 (71.4%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4		20 (100%)		389 (66.5%)						
Acetic acid	64-19-7					959 (21.0%)		284 (28.2%)			
Ammonium acetate	631-61-8									2 (50%)	

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Boric acid	10043-35-3		3 (15%)								
Carbonic acid, dipotassium salt	584-08-7					1159 (25.4%)					
Cristobalite	14464-46-1		20 (100%)		389 (66.5%)						
Formic acid	64-18-6	55 (100%)						293 (29.1%)			
Hemicellulase enzyme	9012-54-8										
Hemicellulase enzyme concentrate	9025-56-3				395 (67.5%)						
Iron(II) sulfate heptahydrate	7782-63-0								7 (50%)		
Magnesium chloride	7786-30-3		20 (100%)		389 (66.5%)						
Magnesium nitrate	10377-60-3		20 (100%)		389 (66.5%)						
Phenolic resin	9003-35-4										
Sodium hypochlorite	7681-52-9					1046 (23.0%)					
Sodium tetraborate decahydrate	1303-96-4		14 (70%)								
Solvent naphtha, petroleum, heavy aliph.	64742-96-7								7 (50%)	2 (50%)	
1-Butoxy-2-propanol	5131-66-8				315 (53.8%)						

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
1-Propanol	71-23-8					1232 (27.0%)					
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-,tetrachloride	138879-94-4			343 (58.6%)							
2-bromo-3-nitrilopropionamide	1113-55-9										
2-Ethylhexanol	104-76-7										83 (43.0052%)
2-Methyl-3(2H)-isothiazolone	2682-20-4		20 (100%)		389 (66.5%)						
2-Propenoic acid, polymer with 2-propenamide	9003-06-9										
Alkenes, C>10 .alpha.-	64743-02-8			241 (18.0%)							
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										50 (25.9%)
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										48 (24.9%)
Benzyldimethyldodecylammonium chloride	139-07-1			268 (20.0%)							

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Benzylhexadecyldimethylammonium chloride	122-18-9			268 (20.0%)							
Boron sodium oxide	1330-43-4				361 (61.7%)						
C10-C16 ethoxylated alcohol	68002-97-1		3 (15%)								
Calcium chloride	10043-52-4		20 (100%)								
Carbon dioxide	124-38-9								7 (50%)		
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	55 (100%)									
Diethylene glycol	111-46-6										
Diethylene glycol monobutyl ether	112-34-5								7 (50%)		
Diethylenetriamine	111-40-0										55 (28.5%)
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8				314 (53.7%)						
Distillates, petroleum, hydrotreated middle	64742-46-7		3 (15%)								
Ethoxylated C12-16 alcohols	68551-12-2										
Ethoxylated C14-15 alcohols	68951-67-7			241 (18.0%)							
Formic acid, potassium salt	590-29-4										

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Glycerin, natural	56-81-5								7 (50%)		
Isotridecanol, ethoxylated	9043-30-5				312 (53.3%)						
Methenamine	100-97-0							298 (29.6%)			
Naphtha, petroleum, hydrotreated heavy	64742-48-9										
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8								9 (64.3%)		
Potassium chloride	7447-40-7								7 (50%)		
Sodium bromate	7789-38-0								7 (50%)		
Sodium perborate tetrahydrate	10486-00-7										
Sulfamic acid	5329-14-6									2 (50%)	
Terpenes and Terpenoids, sweet orange-oil	68647-72-3									2 (50%)	
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2			268 (20.0%)							
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8										

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Thiourea polymer	68527-49-1			384 (28.7%)							
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8										
Trisodium phosphate	7601-54-9						19 (19.6%)				

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

Table C-3b. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, New Mexico to Wyoming (U.S. EPA, 2015c).

Source: (U.S. EPA, 2015c). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Methanol	67-56-1	1012 (90.8%)	1059 (53.3%)	76 (52.1%)	1270 (70.3%)	1633 (68.6%)	12664 (78.5%)	984 (78.5%)	48 (60.8%)	153 (64.0%)	460 (38.4%)
Distillates, petroleum, hydrotreated light	64742-47-8	699 (62.7%)	943 (47.5%)	122 (83.6%)	1270 (70.3%)	1434 (60.2%)	10677 (66.1%)	934 (74.5%)		196 (82.0%)	612 (51.1%)
Ethylene glycol	107-21-1	503 (45.1%)	724 (36.4%)	83 (56.8%)	843 (46.7%)	807 (33.9%)	9591 (59.4%)	1065 (85.0%)	22 (27.8%)	141 (59.0%)	
Isopropanol	67-63-0	695 (62.3%)	739 (37.2%)	71 (48.6%)	764 (42.28%)	735 (30.9%)	7731 (47.9%)	661 (52.8%)	43 (54.4%)	74 (31.0%)	516 (43.1%)

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quartz	14808-60-7	762 (68.3%)	920 (46.3%)	66 (45.2%)	491 (27.2%)		6869 (42.6%)	503 (40.1%)		53 (22.2%)	356 (29.7%)
Sodium hydroxide	1310-73-2	329 (29.5%)	1028 (51.7%)		490 (27.1%)	406 (17.0%)	7371 (45.7%)	466 (37.2%)			688 (57.4%)
Ethanol	64-17-5	529 (47.4%)	545 (27.4%)	87 (59.6%)	838 (46.4%)	388 (16.3%)	3439 (21.3%)		50 (63.3%)	130 (54.3%)	298 (24.9%)
Guar gum	9000-30-0	702 (63.0%)	1094 (55.1%)	74 (50.7%)	457 (25.3%)	538 (22.6%)	6863 (42.5%)	538 (42.9%)		55 (23.0%)	823 (68.7%)
Hydrochloric acid	7647-01-0	880 (78.9%)		145 (99.3%)	1372 (75.9%)	2279 (95.7%)	11424 (70.8%)	1064 (84.9%)	68 (86.1%)	229 (95.8%)	
Peroxydisulfuric acid, diammonium salt	7727-54-0	836 (75.0%)	1089 (54.8%)	93 (63.7%)	713 (39.5%)		8666 (53.7%)	483 (38.5%)		128 (53.6%)	771 (64.4%)
Propargyl alcohol	107-19-7	760 (68.2%)		72 (49.3%)	732 (40.5%)	1371 (57.6%)	6269 (38.8%)	456 (36.4%)	22 (27.8%)	138 (57.7%)	
Glutaraldehyde	111-30-8	632 (56.7%)		105 (71.9%)	989 (54.7%)	819 (34.4%)	6470 (40.1%)			169 (70.7%)	260 (21.7%)
Naphthalene	91-20-3		864 (43.5%)		448 (24.8%)			478 (38.1%)	7 (8.9%)		
2-Butoxyethanol	111-76-2	412 (37.0%)				498 (20.9%)	3898 (24.1%)	663 (52.9%)	70 (88.6%)	62 (25.9%)	
Citric acid	77-92-9	447 (40.1%)		96 (65.8%)	644 (35.6%)	701 (29.4%)	3820 (23.7%)	992 (79.2%)	63 (79.8%)	98 (41.0%)	
Saline	7647-14-5		491 (24.7%)				3462 (21.4%)		7 (8.9%)	53 (22.2%)	274 (22.9%)
Solvent naphtha, petroleum, heavy arom.	64742-94-5		981 (49.4%)		557 (30.8%)		2751 (17.0%)		7 (8.9%)		415 (34.6%)

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1			54 (37.0%)	597 (33.0%)	373 (15.7%)				53 (22.2%)	
2,2-Dibromo-3-nitrilopropionamide	10222-01-2					804 (33.8%)			22 (27.8%)		
Potassium hydroxide	1310-58-3		1176 (59.2%)	106 (72.6%)			6369 (39.5%)				
Choline chloride	67-48-1	384 (34.4%)		55 (37.7%)				649 (51.8%)	45 (57.0%)		
Polyethylene glycol	25322-68-3		567 (28.5%)			688 (28.9%)					
1,2,4-Trimethylbenzene	95-63-6		496 (25.0%)						7 (8.9%)		
Ammonium chloride	12125-02-9					732 (30.7%)				50 (20.9%)	
Diatomaceous earth, calcined	91053-39-3	419 (37.6%)						435 (34.7%)			
Didecyl dimethyl ammonium chloride	7173-51-5			46 (31.6%)						49 (20.5%)	
Sodium chlorite	7758-19-2		482 (24.3%)								271 (22.6%)
Sodium erythorbate	6381-77-7								10 (12.7%)	76 (31.8%)	
N,N-Dimethylformamide	68-12-2			68 (46.6%)	355 (19.6%)			410 (32.7%)			
Nonyl phenol ethoxylate	9016-45-9	333 (29.9%)						447 (35.7%)	25 (31.6%)		

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0								7 (8.9%)		
Sodium persulfate	7775-27-1					373 (15.7%)					308 (25.7%)
Tetramethylammonium chloride	75-57-0		579 (29.1%)								315 (26.3%)
1,2-Propylene glycol	57-55-6								22 (27.8%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4										
Acetic acid	64-19-7										
Ammonium acetate	631-61-8										323 (27.0%)
Boric acid	10043-35-3			82 (56.2%)							
Carbonic acid, dipotassium salt	584-08-7		482 (24.2%)								
Cristobalite	14464-46-1										
Formic acid	64-18-6										
Hemicellulase enzyme	9012-54-8					367 (15.4%)			11 (13.9%)		
Hemicellulase enzyme concentrate	9025-56-3	331 (29.7%)									
Iron(II) sulfate heptahydrate	7782-63-0								22 (27.8%)		
Magnesium chloride	7786-30-3										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Magnesium nitrate	10377-60-3										
Phenolic resin	9003-35-4	419 (37.6%)					2903 (18.0%)				
Sodium hypochlorite	7681-52-9										282 (23.5%)
Sodium tetraborate decahydrate	1303-96-4										265 (22.1%)
Solvent naphtha, petroleum, heavy aliph.	64742-96-7										
1-Butoxy-2-propanol	5131-66-8										
1-Propanol	71-23-8										
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxy ethyl) methylammonio] ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4										
2-Bromo-3-nitrilopropionamide	1113-55-9								11 (13.9%)		
2-Ethylhexanol	104-76-7										
2-Methyl-3(2H)-isothiazolone	2682-20-4										
2-Propenoic acid, polymer with 2-propenamide	9003-06-9							486 (38.8%)			
Alkenes, C>10 .alpha.-	64743-02-8										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										
Benzyldimethyldodecylammonium chloride	139-07-1										
Benzylhexadecyldimethylammonium chloride	122-18-9										
Boron sodium oxide	1330-43-4										
C10-C16 ethoxylated alcohol	68002-97-1										
Calcium chloride	10043-52-4										
Carbon dioxide	124-38-9										
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2										
Diethylene glycol	111-46-6			45 (30.8%)							
Diethylene glycol monobutyl ether	112-34-5										
Diethylenetriamine	111-40-0										
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Distillates, petroleum, hydrotreated middle	64742-46-7										
Ethoxylated C12-16 alcohols	68551-12-2									57 (23.8%)	
Ethoxylated C14-15 alcohols	68951-67-7										
Formic acid, potassium salt	590-29-4										361 (30.1%)
Glycerin, natural	56-81-5										
Isotridecanol, ethoxylated	9043-30-5										
Methenamine	100-97-0										
Naphtha, petroleum, hydrotreated heavy	64742-48-9										384 (32.1%)
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8										
Potassium chloride	7447-40-7										
Sodium bromate	7789-38-0										
Sodium perborate tetrahydrate	10486-00-7				351 (19.4%)						
Sulfamic acid	5329-14-6										
Terpenes and terpenoids, sweet orange-oil	68647-72-3										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2										
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8							945 (75.4%)			
Thiourea polymer	68527-49-1										
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8					350 (14.7%)					
Trisodium phosphate	7601-54-9										

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

Table C-4. Estimated mean, median, 5th percentile, and 95th percentile volumes in gallons for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	2,702	406	0	19,741
1-Butoxy-2-propanol	5131-66-8	167	21	5	654
1-Decanol	112-30-1	28	4	0	33
1-Octanol	111-87-5	5	4	0	10
1-Propanol	71-23-8	128	55	6	367
1,2-Propylene glycol	57-55-6	13,105	72	4	61,071
1,2,4-Trimethylbenzene	95-63-6	38	6	0	43
2-Butoxyethanol	111-76-2	385	26	0	1,811
2-Ethylhexanol	104-76-7	100	11	0	292
2-Mercaptoethanol	60-24-2	1,175	445	0	4,194
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	183	5	0	341
Acetic acid	64-19-7	646	47	0	1,042
Acetic anhydride	108-24-7	239	50	3	722
Acrylamide	79-06-1	95	3	0	57
Adipic acid	124-04-9	153	0	0	109
Aluminum chloride	7446-70-0	2	0	0	0
Ammonia	7664-41-7	44	35	2	138
Ammonium acetate	631-61-8	839	117	0	1,384
Ammonium chloride	12125-02-9	440	48	3	458
Ammonium hydroxide	1336-21-6	7	2	0	14
Benzyl chloride	100-44-7	52	0	0	40
Carbonic acid, dipotassium salt	584-08-7	467	113	0	1,729
Chlorine dioxide	10049-04-4	31	11	0	28
Choline chloride	67-48-1	2,131	290	28	4,364
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	68	3	0	697

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Citric acid	77-92-9	163	20	1	269
Dibromoacetonitrile	3252-43-5	22	13	1	45
Diethylene glycol	111-46-6	168	16	0	102
Diethylenetriamine	111-40-0	92	21	0	207
Dodecane	112-40-3	190	31	0	151
Ethanol	64-17-5	831	121	1	2,645
Ethanolamine	141-43-5	70	30	0	283
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	614	184	4	2,470
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	200	0	0	8
Formic acid	64-18-6	501	38	1	1,229
Fumaric acid	110-17-8	2	0	0	12
Glutaraldehyde	111-30-8	1,313	122	2	1,165
Glycerin, natural	56-81-5	413	109	10	911
Glycolic acid	79-14-1	38	10	4	94
Hydrochloric acid	7647-01-0	28,320	3,110	96	26,877
Isopropanol	67-63-0	2,095	55	0	1,264
Isopropylamine	75-31-0	83	121	0	172
Magnesium chloride	7786-30-3	14	0	0	2
Methanol	67-56-1	1,218	110	2	3,731
Methenamine	100-97-0	3,386	100	0	3,648
Methoxyacetic acid	625-45-6	36	4	2	115
N,N-Dimethylformamide	68-12-2	119	10	0	216
Naphthalene	91-20-3	72	12	0	204
Nitrogen, liquid	7727-37-9	41,841	26,610	3,091	108,200
Ozone	10028-15-6	15,844	15,473	8,785	26,063
Peracetic acid	79-21-0	300	268	50	663
Phosphonic acid	13598-36-2	1,201	0	0	3
Phosphoric acid Divosan X-Tend formulation	7664-38-2	13	4	0	15
Potassium acetate	127-08-2	204	1	0	974

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Propargyl alcohol	107-19-7	183	2	0	51
Saline	7647-14-5	876	85	0	1,544
Saturated sucrose	57-50-1	1	1	0	2
Silica, amorphous	7631-86-9	6,877	8	0	38,371
Sodium carbonate	497-19-8	228	16	0	1,319
Sodium formate	141-53-7	0	0	0	0
Sodium hydroxide	1310-73-2	551	38	0	1,327
Sulfur dioxide	7446-09-5	0	0	0	0
Sulfuric acid	7664-93-9	3	0	0	3
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	156	64	0	557
Tetramethylammonium chloride	75-57-0	970	483	2	3,508
Thioglycolic acid	68-11-1	55	7	2	229
Toluene	108-88-3	18	0	0	11
Tridecane	629-50-5	190	31	0	190
Triethanolamine	102-71-6	846	60	0	2,264
Triethyl phosphate	78-40-0	55	1	0	533
Triethylene glycol	112-27-6	5,198	116	28	945
Triisopropanolamine	122-20-3	46	4	1	330
Trimethyl borate	121-43-7	83	40	4	283
Undecane	1120-21-4	273	29	0	1,641

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-5. Estimated mean, median, 5th percentile, and 95th percentile volumes in liters for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	10,229	1,536	0	74,729
1-Butoxy-2-propanol	5131-66-8	631	80	18	2,475
1-Decanol	112-30-1	107	14	1	123
1-Octanol	111-87-5	21	14	1	39
1-Propanol	71-23-8	483	208	22	1,391
1,2-Propylene glycol	57-55-6	49,607	274	15	231,179
1,2,4-Trimethylbenzene	95-63-6	145	24	0	165
2-Butoxyethanol	111-76-2	1,459	98	0	6,856
2-Ethylhexanol	104-76-7	377	40	1	1,106
2-Mercaptoethanol	60-24-2	4,449	1,685	0	15,878
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	692	18	0	1,292
Acetic acid	64-19-7	2,446	176	0	3,945
Acetic anhydride	108-24-7	906	189	12	2,734
Acrylamide	79-06-1	361	10	0	216
Adipic acid	124-04-9	578	0	0	414
Aluminum chloride	7446-70-0	6	0	0	0
Ammonia	7664-41-7	166	134	7	523
Ammonium acetate	631-61-8	3,177	444	0	5,238
Ammonium chloride	12125-02-9	1,666	182	11	1,733
Ammonium hydroxide	1336-21-6	27	6	1	52
Benzyl chloride	100-44-7	196	1	0	151
Carbonic acid, dipotassium salt	584-08-7	1,769	429	0	6,544
Chlorine dioxide	10049-04-4	117	43	1	106
Choline chloride	67-48-1	8,068	1,096	107	16,521
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	258	12	0	2,638
Citric acid	77-92-9	618	77	5	1,019

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Dibromoacetonitrile	3252-43-5	82	50	4	170
Diethylene glycol	111-46-6	636	61	1	384
Diethylenetriamine	111-40-0	347	80	0	785
Dodecane	112-40-3	719	117	0	572
Ethanol	64-17-5	3,144	458	6	10,011
Ethanolamine	141-43-5	264	112	0	1,070
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	2,324	697	14	9,349
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	756	2	0	31
Formic acid	64-18-6	1,896	144	2	4,653
Fumaric acid	110-17-8	9	0	0	46
Glutaraldehyde	111-30-8	4,972	462	6	4,409
Glycerin, natural	56-81-5	1,565	412	38	3,447
Glycolic acid	79-14-1	146	39	14	356
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741
Isopropanol	67-63-0	7,932	210	1	4,786
Isopropylamine	75-31-0	314	458	0	652
Magnesium chloride	7786-30-3	52	0	0	8
Methanol	67-56-1	4,609	416	6	14,125
Methenamine	100-97-0	12,817	378	0	13,810
Methoxyacetic acid	625-45-6	136	17	8	436
N,N-Dimethylformamide	68-12-2	449	38	2	819
Naphthalene	91-20-3	271	44	0	774
Nitrogen, liquid	7727-37-9	158,384	100,731	11,700	409,583
Ozone	10028-15-6	59,976	58,570	33,254	98,658
Peracetic acid	79-21-0	1,137	1,016	190	2,511
Phosphonic acid	13598-36-2	4,547	2	0	11
Phosphoric acid Divosan X-Tend formulation	7664-38-2	51	15	0	57
Potassium acetate	127-08-2	775	3	0	3,690
Propargyl alcohol	107-19-7	693	9	0	193

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Saline	7647-14-5	3,317	321	0	5,844
Saturated sucrose	57-50-1	5	2	0	6
Silica, amorphous	7631-86-9	26,031	32	0	145,251
Sodium carbonate	497-19-8	862	62	0	4,991
Sodium formate	141-53-7	1	1	0	1
Sodium hydroxide	1310-73-2	2,087	144	1	5,024
Sulfur dioxide	7446-09-5	2	0	0	0
Sulfuric acid	7664-93-9	10	0	0	12
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	591	242	0	2,109
Tetramethylammonium chloride	75-57-0	3,672	1,830	8	13,279
Thioglycolic acid	68-11-1	208	28	6	868
Toluene	108-88-3	69	0	0	41
Tridecane	629-50-5	721	118	0	721
Triethanolamine	102-71-6	3,203	228	0	8,570
Triethyl phosphate	78-40-0	209	6	0	2,019
Triethylene glycol	112-27-6	19,676	439	106	3,579
Triisopropanolamine	122-20-3	174	16	4	1,249
Trimethyl borate	121-43-7	314	152	16	1,072
Undecane	1120-21-4	1,035	111	0	6,212

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-6. Calculated mean, median, 5th percentile, and 95th percentile chemical masses reported to FracFocus in 100 or more disclosures, where density information was available.

Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7. Number of disclosures reported for each chemical is also included.

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	8,593	1,290	0	62,772	578
1-Butoxy-2-propanol	5131-66-8	555	71	16	2,178	773
1-Decanol	112-30-1	89	12	1	102	434
1-Octanol	111-87-5	17	12	1	32	434
1-Propanol	71-23-8	386	167	18	1,113	1,481
1,2-Propylene glycol	57-55-6	51,095	282	15	238,114	1,023
1,2,4-Trimethylbenzene	95-63-6	126	21	0	143	3,976
2-Butoxyethanol	111-76-2	1,313	88	0	6,170	6,778
2-Ethylhexanol	104-76-7	313	34	0	918	1,291
2-Mercaptoethanol	60-24-2	489	185	0	1,747	2,051
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,660	44	0	3,102	4,927
Acetic acid	64-19-7	2,544	183	0	4,103	7,643
Acetic anhydride	108-24-7	969	203	12	2,925	1,377
Acrylamide	79-06-1	408	11	0	244	251
Adipic acid	124-04-9	785	0	0	564	233
Aluminum chloride	7446-70-0	15	0	0	0	122
Ammonia	7664-41-7	111	90	4	351	398
Ammonium acetate	631-61-8	3,718	520	0	6,129	1,504
Ammonium chloride	12125-02-9	2,530	277	16	2,633	3,288
Ammonium hydroxide	1336-21-6	48	11	2	94	1,173
Benzyl chloride	100-44-7	214	1	0	165	1,833
Carbonic acid, dipotassium salt	584-08-7	4,298	1,042	0	15,902	4,093
Chlorine dioxide	10049-04-4	321	117	3	291	331
Choline chloride	67-48-1	9,440	1,282	125	19,329	4,241
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	284	13	0	2,902	1,377

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Citric acid	77-92-9	989	123	8	1,630	7,503
Dibromoacetonitrile	3252-43-5	193	118	11	403	272
Diethylene glycol	111-46-6	712	68	1	430	1,732
Diethylenetriamine	111-40-0	330	76	0	746	784
Dodecane	112-40-3	539	88	0	429	131
Ethanol	64-17-5	2,484	361	4	7,908	9,233
Ethanolamine	141-43-5	267	113	0	1,081	585
Ethyl acetate	141-78-6	0	0	0	0	110
Ethylene glycol	107-21-1	2,557	767	15	10,283	14,767
Ferric chloride	7705-08-0	0	0	0	0	118
Formalin	50-00-0	816	2	0	34	456
Formic acid	64-18-6	2,313	176	2	5,677	3,781
Fumaric acid	110-17-8	15	0	0	75	224
Glutaraldehyde	111-30-8	4,972	462	6	4,409	10,963
Glycerin, natural	56-81-5	1,972	519	47	4,343	1,829
Glycolic acid	79-14-1	217	58	21	530	595
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741	20,996
Isopropanol	67-63-0	6,187	163	1	3,733	15,058
Isopropylamine	75-31-0	213	311	0	444	255
Magnesium chloride	7786-30-3	120	1	0	18	1,113
Methanol	67-56-1	3,641	329	5	11,159	23,225
Methenamine	100-97-0	15,380	454	0	16,572	4,412
Methoxyacetic acid	625-45-6	161	20	9	514	584
N,N-Dimethylformamide	68-12-2	422	36	2	770	2,972
Naphthalene	91-20-3	220	35	0	627	5,945
Nitrogen, liquid	7727-37-9	129,875	82,599	9,594	335,858	713
Ozone	10028-15-6	129	126	71	212	209
Peracetic acid	79-21-0	1,251	1,117	209	2,762	221
Phosphonic acid	13598-36-2	7,730	3	0	18	2,216
Phosphoric acid Divosan X-Tend formulation	7664-38-2	48	14	0	54	315
Potassium acetate	127-08-2	1,216	5	0	5,793	325

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Propargyl alcohol	107-19-7	658	9	0	183	10,771
Saline	7647-14-5	7,197	696	0	12,682	6,673
Saturated sucrose	57-50-1	6	2	0	7	125
Silica, amorphous	7631-86-9	57,267	71	0	319,553	2,423
Sodium carbonate	497-19-8	2,191	158	0	12,678	396
Sodium formate	141-53-7	2	1	1	2	204
Sodium hydroxide	1310-73-2	4,445	306	2	10,701	12,585
Sulfur dioxide	7446-09-5	2	0	0	0	224
Sulfuric acid	7664-93-9	18	0	0	22	402
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	532	218	0	1,898	814
Tetramethylammonium chloride	75-57-0	4,296	2,141	10	15,537	3,162
Thioglycolic acid	68-11-1	277	37	8	1,155	156
Toluene	108-88-3	59	0	0	35	214
Tridecane	629-50-5	541	88	0	541	132
Triethanolamine	102-71-6	3,588	255	0	9,599	1,498
Triethyl phosphate	78-40-0	222	6	0	2,140	991
Triethylene glycol	112-27-6	22,038	491	119	4,008	528
Triisopropanolamine	122-20-3	177	17	4	1,274	251
Trimethyl borate	121-43-7	292	141	14	997	294
Undecane	1120-21-4	766	82	0	4,597	241

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-7. Associated chemical densities and references used to calculate chemical mass and estimate chemical volume.

Name	CASRN	Density (g/mL)	Reference
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	0.84	Dejoye Tanzi et al. (2012)
1-Butoxy-2-propanol	5131-66-8	0.88	Pal et al. (2013)
1-Decanol	112-30-1	0.83	Faria et al. (2013)
1-Octanol	111-87-5	0.82	Dubey and Kumar (2013)
1-Propanol	71-23-8	0.8	Rani and Maken (2013)
1,2-Propylene glycol	57-55-6	1.03	Moosavi et al. (2013)
1,2,4-Trimethylbenzene	95-63-6	0.87	He et al. (2008)
2-Butoxyethanol	111-76-2	0.9	Dhondge et al. (2010)
2-Ethylhexanol	104-76-7	0.83	Laavi et al. (2012)
2-Mercaptoethanol	60-24-2	0.11	Rawat et al. (1976)
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	2.4	Fels (1900)
Acetic acid	64-19-7	1.04	Chafer et al. (2010)
Acetic anhydride	108-24-7	1.07	Radwan and Hanna (1976)
Acrylamide	79-06-1	1.13	Carpenter and Davis (1957)
Adipic acid	124-04-9	1.36	Thalladi et al. (2000)
Aluminum chloride	7446-70-0	2.44	Sigma-Aldrich (2015a)
Ammonia	7664-41-7	0.67	Harlow et al. (1997)
Ammonium acetate	631-61-8	1.17	Biltz and Balz (1928)
Ammonium chloride	12125-02-9	1.519	Haynes (2014)
Ammonium hydroxide	1336-21-6	1.8	Xiao et al. (2013)
Benzyl chloride	100-44-7	1.09	Sarkar et al. (2012)
Carbonic acid, dipotassium salt	584-08-7	2.43	Sigma-Aldrich (2014b)
Chlorine dioxide	10049-04-4	2.757	Haynes (2014)
Choline chloride	67-48-1	1.17	Shanley and Collin (1961)
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	1.1	Masood et al. (1976)
Citric acid	77-92-9	1.6	Bennett and Yuill (1935)
Dibromoacetonitrile	3252-43-5	2.37	Wilt (1956)
Diethylene glycol	111-46-6	1.12	Chasib (2013)
Diethylenetriamine	111-40-0	0.95	Dubey and Kumar (2011)
Dodecane	112-40-3	0.75	Baragi et al. (2013)

Name	CASRN	Density (g/mL)	Reference
Ethanol	64-17-5	0.79	Kiselev et al. (2012)
Ethanolamine	141-43-5	1.01	Blanco et al. (2013)
Ethyl acetate	141-78-6	0.89	Laavi et al. (2013)
Ethylene glycol	107-21-1	1.1	Rodnikova et al. (2012)
Ferric chloride	7705-08-0	2.9	Haynes (2014)
Formalin	50-00-0	1.08	Alfa Aesar (2015)
Formic acid	64-18-6	1.22	Casanova et al. (1981)
Fumaric acid	110-17-8	1.64	Huffman and Fox (1938)
Glutaraldehyde	111-30-8	1	Oka (1962)
Glycerin, natural	56-81-5	1.26	Egorov et al. (2013)
Glycolic acid	79-14-1	1.49	Pijper (1971)
Hydrochloric acid	7647-01-0	1	Steinhauser et al. (1990)
Isopropanol	67-63-0	0.78	Zhang et al. (2013)
Isopropylamine	75-31-0	0.68	Sarkar and Roy (2009)
Magnesium chloride	7786-30-3	2.32	Haynes (2014)
Methanol	67-56-1	0.79	Kiselev et al. (2012)
Methenamine	100-97-0	1.2	Mak (1965)
Methoxyacetic acid	625-45-6	1.18	Haynes (2014)
N,N-Dimethylformamide	68-12-2	0.94	Smirnov and Badelin (2013)
Naphthalene	91-20-3	0.81	Dyshin et al. (2008)
Nitrogen, liquid	7727-37-9	0.8	finemech (2012)
Ozone	10028-15-6	0.002144	Haynes (2014)
Peracetic acid	79-21-0	1.1	Sigma-Aldrich (2015b)
Phosphonic acid	13598-36-2	1.7	Sigma-Aldrich (2014a)
Phosphoric acid Divosan X-Tend formulation	7664-38-2	0.94	Fadeeva et al. (2004)
Potassium acetate	127-08-2	1.57	Haynes (2014)
Propargyl alcohol	107-19-7	0.95	Vijaya Kumar et al. (1996)
Saline	7647-14-5	2.17	Sigma-Aldrich (2010)
Saturated sucrose	57-50-1	1.13	Hagen and Kaatze (2004)
Silica, amorphous	7631-86-9	2.2	Fujino et al. (2004)
Sodium carbonate	497-19-8	2.54	Haynes (2014)
Sodium formate	141-53-7	1.97	Fuess et al. (1982)

Name	CASRN	Density (g/mL)	Reference
Sodium hydroxide	1310-73-2	2.13	Haynes (2014)
Sulfur dioxide	7446-09-5	1.3	Sigma-Aldrich (2015c)
Sulfuric acid	7664-93-9	1.83	Sigma-Aldrich (2015d)
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	0.9	Sigma-Aldrich (2007)
Tetramethylammonium chloride	75-57-0	1.17	Haynes (2014)
Thioglycolic acid	68-11-1	1.33	Biilmann (1906)
Toluene	108-88-3	0.86	Martinez-Reina et al. (2012)
Tridecane	629-50-5	0.75	Zhang et al. (2011)
Triethanolamine	102-71-6	1.12	Blanco et al. (2013)
Triethyl phosphate	78-40-0	1.06	Krakowiak et al. (2001)
Triethylene glycol	112-27-6	1.12	Afzal et al. (2009)
Triisopropanolamine	122-20-3	1.02	IUPAC (2014)
Trimethyl borate	121-43-7	0.93	Sigma-Aldrich (2015e)
Undecane	1120-21-4	0.74	de Oliveira et al. (2011)

Table C-8. Selected physicochemical properties of chemicals reported as used in hydraulic fracturing fluids.

Properties are provided for chemicals, where available from EPI Suite™ version 4.1 (U.S. EPA, 2012a).

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
(13Z)-N,N-bis(2-hydroxyethyl)-N-methyldocos-13-en-1-aminium chloride	120086-58-0	4.38	--	0.3827	3.32×10^{-15}	--	--
(2,3-Dihydroxypropyl)trimethyl ammonium chloride	34004-36-9	-5.8	--	1.00×10^{6}	9.84×10^{-18}	--	--
(E)-Crotonaldehyde	123-73-9	0.6	--	4.15×10^{4}	5.61×10^{-5}	1.90×10^{-5}	1.94×10^{-5}
[Nitrilotris(methylene)]tris-phosphonic acid pentasodium salt	2235-43-0	−5.45	−3.53	1.00×10^{6}	1.65×10^{-34}	--	--
1-(1-Naphthylmethyl)quinolinium chloride	65322-65-8	5.57	--	0.02454	1.16×10^{-7}	--	--
1-(Alkyl* amino)-3-aminopropane *(42%C12, 26%C18, 15%C14, 8%C16, 5%C10, 4%C8)	68155-37-3	4.74	--	23.71	6.81×10^{-8}	2.39×10^{-8}	--
1-(Phenylmethyl)pyridinium Et Me derivatives, chlorides	68909-18-2	4.1	--	14.13	1.78×10^{-5}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1,2,3-Trimethylbenzene	526-73-8	3.63	3.66	75.03	7.24×10^{-3}	6.58×10^{-3}	4.36×10^{-3}
1,2,4-Trimethylbenzene	95-63-6	3.63	3.63	79.59	7.24×10^{-3}	6.58×10^{-3}	6.16×10^{-3}
1,2-Benzisothiazolin-3-one	2634-33-5	0.64	--	2.14×10^{4}	6.92×10^{-9}	--	--
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	1.63	--	424	3.94×10^{-10}	--	--
1,2-Dimethylbenzene	95-47-6	3.09	3.12	224.1	6.56×10^{-3}	6.14×10^{-3}	5.18×10^{-3}
1,2-Ethanediaminium, N,N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4	−23.19	--	1.00×10^{6}	2.33×10^{-35}	--	--
1,2-Propylene glycol	57-55-6	-0.78	−0.92	8.11×10^{5}	1.74×10^{-7}	1.31×10^{-10}	1.29×10^{-8}
1,2-Propylene oxide	75-56-9	0.37	0.03	1.29×10^{5}	1.60×10^{-4}	1.23×10^{-4}	6.96×10^{-5}
1,3,5-Triazine	290-87-9	−0.2	0.12	1.03×10^{5}	1.21×10^{-6}	--	--
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	−4.67	--	1.00×10^{6}	1.08×10^{-11}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1,3,5-Trimethylbenzene	108-67-8	3.63	3.42	120.3	7.24×10^{-3}	6.58×10^{-3}	8.77×10^{-3}
1,3-Butadiene	106-99-0	2.03	1.99	792.3	7.79×10^{-2}	7.05×10^{-2}	7.36×10^{-2}
1,3-Dichloropropene	542-75-6	2.29	2.04	1,994	2.45×10^{-2}	3.22×10^{-3}	3.55×10^{-3}
1,4-Dioxane	123-91-1	−0.32	−0.27	2.14×10^{5}	5.91×10^{-6}	1.12×10^{-7}	4.80×10^{-6}
1,6-Hexanediamine	124-09-4	0.35	--	5.34×10^{5}	3.21×10^{-9}	7.05×10^{-10}	--
1,6-Hexanediamine dihydrochloride	6055-52-3	0.35	--	5.34×10^{5}	3.21×10^{-9}	7.05×10^{-10}	--
1-[2-(2-Methoxy-1-methylethoxy)-1-methylethoxy]-2-propanol	20324-33-8	−0.2	--	1.96×10^{5}	2.36×10^{-11}	4.55×10^{-13}	--
1-Amino-2-propanol	78-96-6	−1.19	−0.96	1.00×10^{6}	4.88×10^{-10}	2.34×10^{-10}	--
1-Benzylquinolinium chloride	15619-48-4	4.4	--	6.02	1.19×10^{-6}	--	--
1-Butanol	71-36-3	0.84	0.88	7.67×10^{4}	9.99×10^{-6}	9.74×10^{-6}	8.81×10^{-6}
1-Butoxy-2-propanol	5131-66-8	0.98	--	4.21×10^{4}	1.30×10^{-7}	4.88×10^{-8}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Decanol	112-30-1	3.79	4.57	28.21	5.47×10^{-5}	7.73×10^{-5}	3.20×10^{-5}
1-Dodecyl-2-pyrrolidinone	2687-96-9	5.3	4.2	5.862	7.12×10^{-7}	--	--
1-Eicosene	3452-07-1	10.03	--	1.26×10^{-5}	1.89×10^{1}	6.74×10^{1}	--
1-Ethyl-2-methylbenzene	611-14-3	3.58	3.53	96.88	8.71×10^{-3}	9.52×10^{-3}	5.53×10^{-3}
1-Hexadecene	629-73-2	8.06	--	0.001232	6.10	1.69×10^{1}	--
1-Hexanol	111-27-3	1.82	2.03	6,885	1.76×10^{-5}	1.94×10^{-5}	1.71×10^{-5}
1-Methoxy-2-propanol	107-98-2	−0.49	--	1.00×10^{6}	5.56×10^{-8}	1.81×10^{-8}	9.20×10^{-7}
1-Octadecanamine, acetate (1:1)	2190-04-7	7.71	--	0.04875	9.36×10^{-4}	2.18×10^{-3}	--
1-Octadecanamine, N,N-dimethyl-	124-28-7	8.39	--	0.008882	4.51×10^{-3}	3.88×10^{-2}	--
1-Octadecene	112-88-9	9.04	--	1.256×10^{-4}	10.7	3.38×10^{1}	--
1-Octanol	111-87-5	2.81	3	814	3.10×10^{-5}	3.88×10^{-5}	2.45×10^{-5}
1-Pentanol	71-41-0	1.33	1.51	2.09×10^{4}	1.33×10^{-5}	1.38×10^{-5}	1.30×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3327-22-8	−4.48	--	1.00×10^{6}	9.48×10^{-17}	--	--
1-Propanesulfonic acid	5284-66-2	−1.4	--	1.00×10^{6}	2.22×10^{-8}	--	--
1-Propanol	71-23-8	0.35	0.25	2.72×10^{5}	7.52×10^{-6}	6.89×10^{-6}	7.41×10^{-6}
1-Propene	115-07-1	1.68	1.77	1,162	1.53×10^{-1}	1.58×10^{-1}	1.96×10^{-1}
1-tert-Butoxy-2-propanol	57018-52-7	0.87	--	5.24×10^{4}	1.30×10^{-7}	5.23×10^{-8}	--
1-Tetradecene	1120-36-1	7.08	--	0.01191	3.46	8.48	--
1-Tridecanol	112-70-9	5.26	--	4.533	1.28×10^{-4}	2.18×10^{-4}	--
1-Undecanol	112-42-5	4.28	--	43.04	7.26×10^{-5}	1.09×10^{-4}	--
2-(2-Butoxyethoxy)ethanol	112-34-5	0.29	0.56	7.19×10^{4}	1.52×10^{-9}	4.45×10^{-11}	7.20×10^{-9}
2-(2-Ethoxyethoxy)ethanol	111-90-0	−0.69	−0.54	8.28×10^{5}	8.63×10^{-10}	2.23×10^{-11}	2.23×10^{-8}
2-(2-Ethoxyethoxy)ethyl acetate	112-15-2	0.32	--	3.09×10^{4}	5.62×10^{-8}	7.22×10^{-10}	2.29×10^{-8}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-(Dibutylamino)ethanol	102-81-8	2.01	2.65	3,297	9.70×10^{-9}	1.02×10^{-8}	--
2-(Hydroxymethylamino)ethanol	34375-28-5	−1.53	--	1.00×10^{6}	1.62×10^{-12}	--	--
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	3.12	3.3	41.67	6.49×10^{-12}	--	--
2,2'-(Diazene-1,2-diyldiethane-1,1-diyl)bis-4,5-dihydro-1H-imidazole dihydrochloride	27776-21-2	2.12	--	193.3	3.11×10^{-14}	--	--
2,2'-(Octadecylimino)diethanol	10213-78-2	6.85	--	0.08076	1.06×10^{-8}	7.39×10^{-12}	--
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	−2.17	--	1.00×10^{6}	2.50×10^{-13}	8.10×10^{-16}	--
2,2'-Azobis(2-amidinopropane) dihydrochloride	2997-92-4	−3.28	--	1.00×10^{6}	1.21×10^{-14}	--	--
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1.01	0.82	2,841	6.16×10^{-14}	--	1.91×10^{-8}
2,2-Dibromopropanediamide	73003-80-2	0.37	--	1.00×10^{4}	3.58×10^{-14}	--	--
2,4-Hexadienoic acid, potassium salt, (2E,4E)-	24634-61-5	1.62	1.33	1.94×10^{4}	5.72×10^{-7}	4.99×10^{-8}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2,6,8-Trimethyl-4-nonanol	123-17-1	4.48	--	24.97	9.63×10^{-5}	4.45×10^{-4}	--
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	−2.19	--	1.00×10^{6}	5.18×10^{-15}	--	--
2-Amino-2-methylpropan-1-ol	124-68-5	−0.74	--	1.00×10^{6}	6.48×10^{-10}	--	--
2-Aminoethanol hydrochloride	2002-24-6	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
2-Bromo-3-nitrilopropionamide	1113-55-9	−0.31	--	3,274	5.35×10^{-13}	--	--
2-Butanone oxime	96-29-7	1.69	0.63	3.66×10^{4}	1.04×10^{-5}	--	--
2-Butoxy-1-propanol	15821-83-7	0.98	--	4.21×10^{4}	1.30×10^{-7}	4.88×10^{-8}	--
2-Butoxyethanol	111-76-2	0.57	0.83	6.45×10^{4}	9.79×10^{-8}	2.08×10^{-8}	1.60×10^{-6}
2-Dodecylbenzenesulfonic acid- N-(2-aminoethyl)ethane-1,2-diamine(1:1)	40139-72-8	4.78	--	0.7032	6.27×10^{-8}	--	--
2-Ethoxyethanol	110-80-5	−0.42	−0.32	7.55×10^{5}	5.56×10^{-8}	1.04×10^{-8}	4.70×10^{-7}
2-Ethoxynaphthalene	93-18-5	3.74	--	38.32	4.13×10^{-5}	4.06×10^{-4}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-Ethyl-1-hexanol	104-76-7	2.73	--	1,379	3.10×10^{-5}	4.66×10^{-5}	2.65×10^{-5}
2-Ethyl-2-hexenal	645-62-5	2.62	--	548.6	2.06×10^{-4}	4.88×10^{-4}	--
2-Ethylhexyl benzoate	5444-75-7	5.19	--	1.061	2.52×10^{-4}	2.34×10^{-4}	--
2-Hydroxyethyl acrylate	818-61-1	−0.25	−0.21	5.07×10^{5}	4.49×10^{-9}	7.22×10^{-10}	--
2-Hydroxyethylammonium hydrogen sulphite	13427-63-9	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	7006-59-9	−6.7	--	1.00×10^{6}	4.78×10^{-19}	--	--
2-Mercaptoethanol	60-24-2	−0.2	--	1.94×10^{5}	1.27×10^{-7}	3.38×10^{-8}	1.80×10^{-7}
2-Methoxyethanol	109-86-4	−0.91	−0.77	1.00×10^{6}	4.19×10^{-8}	7.73×10^{-9}	3.30×10^{-7}
2-Methyl-1-propanol	78-83-1	0.77	0.76	9.71×10^{4}	9.99×10^{-6}	1.17×10^{-5}	9.78×10^{-6}
2-Methyl-2,4-pentanediol	107-41-5	0.58	--	3.26×10^{4}	4.06×10^{-7}	3.97×10^{-10}	--
2-Methyl-3(2H)-isothiazolone	2682-20-4	−0.83	--	5.37×10^{5}	4.96×10^{-8}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-Methyl-3-butyn-2-ol	115-19-5	0.45	0.28	2.40×10^{5}	1.04×10^{-6}	--	3.91×10^{-6}
2-Methylbutane	78-78-4	2.72	--	184.6	1.29	1.44	1.40
2-Methylquinoline hydrochloride	62763-89-7	2.69	2.59	498.5	7.60×10^{-7}	2.13×10^{-6}	--
2-Phosphono-1,2,4-butanetricarboxylic acid	37971-36-1	−1.66	--	1.00×10^{6}	1.17×10^{-26}	--	--
2-Phosphonobutane-1,2,4-tricarboxylic acid, potassium salt (1:x)	93858-78-7	−1.66	--	1.00×10^{6}	1.17×10^{-26}	--	--
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	13533-05-6	−0.52	−0.3	3.99×10^{5}	6.98×10^{-11}	1.54×10^{-12}	--
3-(Dimethylamino)propylamine	109-55-7	−0.45	--	1.00×10^{6}	6.62×10^{-9}	4.45×10^{-9}	--
3,4,4-Trimethyloxazolidine	75673-43-7	0.13	--	8.22×10^{5}	6.63×10^{-6}	--	--
3,5,7-Triazatricyclo(3.3.1.13,7))decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-	51229-78-8	−5.92	--	1.00×10^{6}	1.76×10^{-8}	--	--
3,7-Dimethyl-2,6-octadienal	5392-40-5	3.45	--	84.71	3.76×10^{-4}	4.35×10^{-5}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
3-Hydroxybutanal	107-89-1	−0.72	--	1.00×10^{6}	4.37×10^{-9}	2.28×10^{-9}	--
3-Methoxypropylamine	5332-73-0	−0.42	--	1.00×10^{6}	1.56×10^{-7}	1.94×10^{-8}	--
3-Phenylprop-2-enal	104-55-2	1.82	1.9	2,150	1.60×10^{-6}	3.38×10^{-7}	--
4,4-Dimethyloxazolidine	51200-87-4	−0.08	--	1.00×10^{6}	3.02×10^{-6}	--	--
4,6-Dimethyl-2-heptanone	19549-80-5	2.56	--	528.8	2.71×10^{-4}	4.55×10^{-4}	--
4-[Abieta-8,11,13-trien-18-yl(3-oxo-3-phenylpropyl)amino]butan-2-one hydrochloride	143106-84-7	7.72	--	0.002229	2.49×10^{-12}	1.20×10^{-14}	--
4-Ethyloct-1-yn-3-ol	5877-42-9	2.87	--	833.9	4.27×10^{-6}	--	--
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	1.05	1.21	6,875	8.27×10^{-11}	2.81×10^{-9}	2.15×10^{-9}
4-Methoxybenzyl formate	122-91-8	1.61	--	2,679	1.15×10^{-6}	2.13×10^{-6}	--
4-Methoxyphenol	150-76-5	1.59	1.58	1.65×10^{4}	3.32×10^{-8}	5.35×10^{-7}	--
4-Methyl-2-pentanol	108-11-2	1.68	--	1.38×10^{4}	1.76×10^{-5}	3.88×10^{-5}	4.45×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
4-Methyl-2-pentanone	108-10-1	1.16	1.31	8,888	1.16×10^{-4}	1.34×10^{-4}	1.38×10^{-4}
4-Nonylphenol	104-40-5	5.99	5.76	1.57	5.97×10^{-6}	1.23×10^{-5}	3.40×10^{-5}
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	−0.34	--	1.49×10^{5}	3.57×10^{-8}	--	--
Acetaldehyde	75-07-0	−0.17	−0.34	2.57×10^{5}	6.78×10^{-5}	6.00×10^{-5}	6.67×10^{-5}
Acetic acid	64-19-7	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Acetic acid, C6-8-branched alkyl esters	90438-79-2	3.25	--	117.8	9.60×10^{-4}	1.07×10^{-3}	--
Acetic acid, hydroxy-, reaction products with triethanolamine	68442-62-6	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}
Acetic acid, mercapto-, monoammonium salt	5421-46-5	0.03	0.09	2.56×10^{5}	1.94×10^{-8}	--	--
Acetic anhydride	108-24-7	−0.58	--	3.59×10^{5}	3.57×10^{-5}	--	5.71×10^{-6}
Acetone	67-64-1	−0.24	−0.24	2.20×10^{5}	4.96×10^{-5}	3.97×10^{-5}	3.50×10^{-5}
Acetonitrile, 2,2',2''-nitrilotris-	7327-60-8	−1.39	--	1.00×10^{6}	2.61×10^{-15}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Acetophenone	98-86-2	1.67	1.58	4,484	9.81×10^{-6}	1.09×10^{-5}	1.04×10^{-5}
Acetyltriethyl citrate	77-89-4	1.34	--	688.2	6.91×10^{-11}	--	--
Acrolein	107-02-8	0.19	−0.01	1.40×10^{5}	3.58×10^{-5}	1.94×10^{-5}	1.22×10^{-4}
Acrylamide	79-06-1	−0.81	−0.67	5.04×10^{5}	5.90×10^{-9}	--	1.70×10^{-9}
Acrylic acid	79-10-7	0.44	0.35	1.68×10^{5}	2.89×10^{-7}	1.17×10^{-7}	3.70×10^{-7}
Acrylic acid, with sodium-2-acrylamido-2-methyl-1-propanesulfonate and sodium phosphinate	110224-99-2	−2.19	--	1.00×10^{6}	5.18×10^{-15}	--	--
Alcohols, C10-12, ethoxylated	67254-71-1	5.47	--	0.9301	1.95×10^{-2}	2.03×10^{-2}	--
Alcohols, C11-14-iso-, C13-rich	68526-86-3	5.19	--	5.237	1.28×10^{-4}	2.62×10^{-4}	--
Alcohols, C11-14-iso-, C13-rich, ethoxylated	78330-21-9	4.91	--	5.237	1.25×10^{-6}	7.73×10^{-7}	--
Alcohols, C12-13, ethoxylated	66455-14-9	5.96	--	0.2995	2.58×10^{-2}	2.87×10^{-2}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Alcohols, C12-14, ethoxylated propoxylated	68439-51-0	6.67	--	0.02971	7.08×10^{-4}	1.23×10^{-4}	--
Alcohols, C12-14-secondary	126950-60-5	5.19	--	5.237	1.28×10^{-4}	3.62×10^{-4}	--
Alcohols, C12-16, ethoxylated	68551-12-2	6.45	--	0.09603	3.43×10^{-2}	4.06×10^{-2}	--
Alcohols, C14-15, ethoxylated	68951-67-7	7.43	--	0.009765	6.04×10^{-2}	8.10×10^{-2}	--
Alcohols, C6-12, ethoxylated	68439-45-2	4.49	--	8.832	1.10×10^{-2}	1.02×10^{-2}	--
Alcohols, C7-9-iso-, C8-rich, ethoxylated	78330-19-5	2.46	--	1,513	3.04×10^{-7}	1.38×10^{-7}	--
Alcohols, C9-11, ethoxylated	68439-46-3	4.98	--	2.874	1.47×10^{-2}	1.44×10^{-2}	--
Alcohols, C9-11-iso-, C10-rich, ethoxylated	78330-20-8	4.9	--	3.321	1.47×10^{-2}	2.39×10^{-2}	--
Alkanes, C12-14-iso-	68551-19-9	6.65	--	0.03173	1.24×10^{1}	2.28×10^{1}	--
Alkanes, C13-16-iso-	68551-20-2	7.63	--	0.003311	2.19×10^{1}	4.55×10^{1}	--
Alkenes, C>10 alpha-	64743-02-8	8.55	--	0.0003941	8.09	2.39×10^{1}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Alkyl* dimethyl ethylbenzyl ammonium chloride *(50%C12, 30%C14, 17%C16, 3%C18)	85409-23-0_1	3.97	--	3.23	1.11×10^{-11}	--	--
Alkyl* dimethyl ethylbenzyl ammonium chloride *(60%C14, 30%C16, 5%C12, 5%C18)	68956-79-6	4.95	--	0.3172	1.96×10^{-11}	--	--
Alkylbenzenesulfonate, linear	42615-29-2	4.71	--	0.8126	6.27×10^{-8}	--	--
alpha-Lactose monohydrate	5989-81-1	−5.12	--	1.00×10^{6}	4.47×10^{-22}	9.81×10^{-45}	--
alpha-Terpineol	98-55-5	3.33	2.98	371.7	1.58×10^{-5}	3.15×10^{-6}	1.22×10^{-5}
Amaranth	915-67-3	1.63	--	1.789	1.49×10^{-30}	--	--
Aminotrimethylene phosphonic acid	6419-19-8	−5.45	−3.53	1.00×10^{6}	1.65×10^{-34}	--	--
Ammonium acetate	631-61-8	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Ammonium acrylate	10604-69-0	0.44	0.35	1.68×10^{5}	2.89×10^{-7}	1.17×10^{-7}	3.70×10^{-7}
Ammonium citrate (1:1)	7632-50-0	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ammonium citrate (2:1)	3012-65-5	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Ammonium dodecyl sulfate	2235-54-3	2.42	--	163.7	1.84×10^{-7}	--	--
Ammonium hydrogen carbonate	1066-33-7	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Ammonium lactate	515-98-0	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Anethole	104-46-1	3.39	--	98.68	2.56×10^{-4}	2.23×10^{-3}	--
Aniline	62-53-3	1.08	0.9	2.08×10^{4}	1.90×10^{-6}	2.18×10^{-6}	2.02×10^{-6}
Benactyzine hydrochloride	57-37-4	2.89	--	292.1	2.07×10^{-10}	--	--
Benzamorf	12068-08-5	4.71	--	0.8126	6.27×10^{-8}	--	--
Benzene	71-43-2	1.99	2.13	2,000	5.39×10^{-3}	5.35×10^{-3}	5.55×10^{-3}
Benzene, C10-16-alkyl derivatives	68648-87-3	8.43	9.36	0.0002099	1.78×10^{-1}	3.97×10^{-1}	--
Benzenesulfonic acid	98-11-3	−1.17	--	6.90×10^{5}	2.52×10^{-9}	--	--
Benzenesulfonic acid, (1-methylethyl)-,	37953-05-2	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Benzenesulfonic acid, (1-methylethyl)-, ammonium salt	37475-88-0	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--
Benzenesulfonic acid, (1-methylethyl)-, sodium salt	28348-53-0	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with cyclohexylamine	255043-08-4	4.71	--	0.8126	6.27×10^{-8}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with triethanolamine	68584-25-8	5.2	--	0.255	8.32×10^{-8}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, potassium salts	68584-27-0	5.2	--	0.255	8.32×10^{-8}	--	--
Benzenesulfonic acid, dodecyl-, branched, compounds with 2-propanamine	90218-35-2	4.49	--	1.254	6.27×10^{-8}	--	--
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, sodium salts	68081-81-2	4.22	--	2.584	4.72×10^{-8}	--	--
Benzoic acid	65-85-0	1.87	1.87	2,493	1.08×10^{-7}	4.55×10^{-8}	3.81×10^{-8}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Benzyl chloride	100-44-7	2.79	2.3	1,030	2.09×10^{-3}	3.97×10^{-4}	4.12×10^{-4}
Benzyldimethyldodecylammonium chloride	139-07-1	2.93	--	36.47	7.61×10^{-12}	--	--
Benzylhexadecyldimethylammonium chloride	122-18-9	4.89	--	0.3543	2.36×10^{-11}	--	--
Benzyltrimethylammonium chloride	56-93-9	−2.47	--	1.00×10^{6}	3.37×10^{-13}	--	--
Bicine	150-25-4	−3.27	--	3.52×10^{5}	1.28×10^{-14}	--	--
Bis(1-methylethyl)naphthalenesulfonic acid, cyclohexylamine salt	68425-61-6	2.92	--	43.36	9.29×10^{-10}	--	--
Bis(2-chloroethyl) ether	111-44-4	1.56	1.29	6,435	1.89×10^{-4}	4.15×10^{-7}	1.70×10^{-5}
Bisphenol A	80-05-7	3.64	3.32	172.7	9.16×10^{-12}	--	--
Bronopol	52-51-7	−1.51	--	8.37×10^{5}	6.35×10^{-21}	--	--
Butane	106-97-8	2.31	2.89	135.6	9.69×10^{-1}	8.48×10^{-1}	9.50×10^{-1}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	2373-38-8	3.98	--	0.1733	1.61×10^{-12}	--	--
Butene	25167-67-3	2.17	2.4	354.8	2.03×10^{-1}	2.68×10^{-1}	2.33×10^{-1}
Butyl glycidyl ether	2426-08-6	1.08	0.63	2.66×10^{4}	4.37×10^{-6}	5.23×10^{-7}	2.47×10^{-5}
Butyl lactate	138-22-7	0.8	--	5.30×10^{4}	8.49×10^{-5}	--	1.92×10^{-6}
Butyryl trihexyl citrate	82469-79-2	8.21	--	5.56×10^{-5}	3.65×10^{-9}	--	--
C.I. Acid Red 1	3734-67-6	0.51	--	6.157	3.73×10^{-29}	--	--
C.I. Acid Violet 12, disodium salt	6625-46-3	0.59	--	3.379	2.21×10^{-30}	--	--
C.I. Pigment Red 5	6410-41-9	7.65	--	4.38×10^{-5}	4.36×10^{-21}	--	--
C.I. Solvent Red 26	4477-79-6	9.27	--	5.68×10^{-5}	5.48×10^{-13}	4.66×10^{-13}	--
C10-16-Alkyldimethylamines oxides	70592-80-2	2.87	--	89.63	1.14×10^{-13}	--	--
C10-C16 Ethoxylated alcohol	68002-97-1	4.99	--	4.532	1.25×10^{-6}	4.66×10^{-7}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
C12-14 tert-Alkyl ethoxylated amines	73138-27-9	3.4	--	264.2	1.29×10^{-10}	--	--
Calcium dodecylbenzene sulfonate	26264-06-2	4.71	--	0.8126	6.27×10^{-8}	--	--
Camphor	76-22-2	3.04	2.38	339.1	7.00×10^{-5}	--	8.10×10^{-5}
Carbon dioxide	124-38-9	0.83	0.83	2.57×10^{4}	1.52×10^{-2}	--	1.52×10^{-2}
Carbonic acid, dipotassium salt	584-08-7	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Choline bicarbonate	78-73-9	−5.16	--	1.00×10^{6}	2.03×10^{-16}	--	--
Choline chloride	67-48-1	−5.16	--	1.00×10^{6}	2.03×10^{-16}	--	--
Citric acid	77-92-9	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Citronellol	106-22-9	3.56	3.91	105.5	5.68×10^{-5}	2.13×10^{-5}	--
Coconut trimethylammonium chloride	61789-18-2	1.22	--	2,816	9.42×10^{-11}	--	--
Coumarin	91-64-5	1.51	1.39	5,126	6.95×10^{-6}	--	9.92×10^{-8}
Cumene	98-82-8	3.45	3.66	75.03	1.05×10^{-2}	1.23×10^{-2}	1.15×10^{-2}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Cyclohexane	110-82-7	3.18	3.44	43.02	2.55×10^{-1}	1.94×10^{-1}	1.50×10^{-1}
Cyclohexanol	108-93-0	1.64	1.23	3.37×10^{4}	4.90×10^{-6}	3.70×10^{-6}	4.40×10^{-6}
Cyclohexanone	108-94-1	1.13	0.81	2.41×10^{4}	5.11×10^{-5}	1.28×10^{-5}	9.00×10^{-6}
Cyclohexylamine sulfate	19834-02-7	1.63	1.49	6.40×10^{4}	1.38×10^{-5}	--	4.16×10^{-6}
D&C Red no. 28	18472-87-2	9.62	--	1.64×10^{-8}	6.37×10^{-21}	--	--
D&C Red no. 33	3567-66-6	0.48	--	11.87	1.15×10^{-26}	--	--
Daidzein	486-66-8	2.55	--	568.4	3.91×10^{-16}	--	--
Dapsone	80-08-0	0.77	0.97	3,589	3.11×10^{-14}	--	--
Dazomet	533-74-4	0.94	0.63	1.94×10^{4}	2.84×10^{-3}	--	4.98×10^{-10}
Decyldimethylamine	1120-24-7	4.46	--	82.23	4.68×10^{-4}	2.45×10^{-3}	--
D-Glucitol	50-70-4	−3.01	−2.2	1.00×10^{6}	7.26×10^{-13}	2.94×10^{-29}	--
D-Gluconic acid	526-95-4	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
D-Glucopyranoside, methyl	3149-68-6	−2.5	--	1.00×10^{6}	1.56×10^{-14}	2.23×10^{-24}	--
D-Glucose	50-99-7	−2.89	−3.24	1.00×10^{6}	9.72×10^{-15}	1.62×10^{-26}	--
Di(2-ethylhexyl) phthalate	117-81-7	8.39	7.6	0.001132	1.18×10^{-5}	1.02×10^{-5}	2.70×10^{-7}
Dibromoacetonitrile	3252-43-5	0.47	--	9,600	4.06×10^{-7}	--	--
Dichloromethane	75-09-2	1.34	1.25	1.10×10^{4}	9.14×10^{-3}	3.01×10^{-3}	3.25×10^{-3}
Didecyldimethylammonium chloride	7173-51-5	4.66	--	0.9	6.85×10^{-10}	--	--
Diethanolamine	111-42-2	−1.71	−1.43	1.00×10^{6}	3.92×10^{-11}	3.46×10^{-15}	3.87×10^{-11}
Diethylbenzene	25340-17-4	4.07	3.72	58.86	1.16×10^{-2}	1.47×10^{-2}	2.61×10^{-3}
Diethylene glycol	111-46-6	−1.47	--	1.00×10^{6}	2.03×10^{-9}	1.20×10^{-13}	--
Diethylene glycol monomethyl ether	111-77-3	−1.18	--	1.00×10^{6}	6.50×10^{-10}	1.65×10^{-11}	--
Diethylenetriamine	111-40-0	−2.13	--	1.00×10^{6}	3.10×10^{-13}	1.09×10^{-14}	--
Diisobutyl ketone	108-83-8	2.56	--	528.8	2.71×10^{-4}	4.55×10^{-4}	1.17×10^{-4}

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Diisopropanolamine	110-97-4	−0.88	−0.82	1.00×10^{6}	6.91×10^{-11}	1.90×10^{-14}	--
Diisopropylnaphthalene	38640-62-9	6.08	--	0.2421	1.99×10^{-3}	1.94×10^{-3}	--
Dimethyl adipate	627-93-0	1.39	1.03	7,749	9.77×10^{-7}	1.28×10^{-7}	2.31×10^{-6}
Dimethyl glutarate	1119-40-0	0.9	0.62	2.02×10^{4}	7.36×10^{-7}	9.09×10^{-8}	6.43×10^{-7}
Dimethyl succinate	106-65-0	0.4	0.35	3.96×10^{4}	5.54×10^{-7}	6.43×10^{-8}	--
Dimethylaminoethanol	108-01-0	−0.94	--	1.00×10^{6}	1.77×10^{-9}	1.77×10^{-9}	3.73×10^{-7}
Dimethyldiallylammonium chloride	7398-69-8	−2.49	--	1.00×10^{6}	7.20×10^{-12}	--	--
Diphenyl oxide	101-84-8	4.05	4.21	15.58	1.18×10^{-4}	2.81×10^{-4}	2.79×10^{-4}
Dipropylene glycol	25265-71-8	−0.64	--	3.11×10^{5}	3.58×10^{-9}	6.29×10^{-10}	--
Di-sec-butylphenol	31291-60-8	5.41	--	3.723	3.74×10^{-6}	6.89×10^{-6}	--
Disodium dodecyl(sulphonatophenoxy)benzenesulphonate	28519-02-0	5.05	--	0.0353	6.40×10^{-16}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Disodium ethylenediaminediacetate	38011-25-5	−4.79	--	1.00×10^{6}	1.10×10^{-16}	--	--
Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
D-Lactic acid	10326-41-7	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
D-Limonene	5989-27-5	4.83	4.57	4.581	3.80×10^{-1}	--	3.19×10^{-2}
Docusate sodium	577-11-7	6.1	--	0.001227	5.00×10^{-12}	--	--
Dodecane	112-40-3	6.23	6.1	0.1099	9.35	1.34×10^{1}	8.18
Dodecylbenzene	123-01-3	7.94	8.65	0.001015	1.34×10^{-1}	2.81×10^{-1}	--
Dodecylbenzenesulfonic acid	27176-87-0	4.71	--	0.8126	6.27×10^{-8}	--	--
Dodecylbenzenesulfonic acid, monoethanolamine salt	26836-07-7	4.71	--	0.8126	6.27×10^{-8}	--	--
Epichlorohydrin	106-89-8	0.63	0.45	5.06×10^{4}	5.62×10^{-5}	2.62×10^{-6}	3.04×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	44992-01-0	−3.1	--	1.00×10^{6}	6.96×10^{-15}	--	--
Ethane	74-84-0	1.32	1.81	938.6	5.50×10^{-1}	4.25×10^{-1}	5.00×10^{-1}
Ethanol	64-17-5	−0.14	−0.31	7.92×10^{5}	5.67×10^{-6}	4.88×10^{-6}	5.00×10^{-6}
Ethanol, 2,2',2''-nitrilotris-, tris(dihydrogen phosphate) (ester), sodium salt	68171-29-9	−3.13	--	1.00×10^{6}	3.08×10^{-36}	--	--
Ethanol, 2-[2-[2-(tridecyloxy) ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	25446-78-0	2.09	--	42	9.15×10^{-13}	--	--
Ethanolamine	141-43-5	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
Ethoxylated dodecyl alcohol	9002-92-0	4.5	--	14.19	9.45×10^{-7}	3.30×10^{-7}	--
Ethyl acetate	141-78-6	0.86	0.73	2.99×10^{4}	2.33×10^{-4}	1.58×10^{-4}	1.34×10^{-4}
Ethyl acetoacetate	141-97-9	−0.2	0.25	5.62×10^{4}	1.57×10^{-7}	--	1.20×10^{-6}
Ethyl benzoate	93-89-0	2.32	2.64	421.5	4.61×10^{-5}	2.45×10^{-5}	7.33×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ethyl lactate	97-64-3	−0.18	--	4.73×10^{5}	4.82×10^{-5}	--	5.83×10^{-7}
Ethyl salicylate	118-61-6	3.09	2.95	737.1	6.04×10^{-6}	3.01×10^{-9}	--
Ethylbenzene	100-41-4	3.03	3.15	228.6	7.89×10^{-3}	8.88×10^{-3}	7.88×10^{-3}
Ethylene	74-85-1	1.27	1.13	3,449	9.78×10^{-2}	1.62×10^{-1}	2.28×10^{-1}
Ethylene glycol	107-21-1	−1.2	−1.36	1.00×10^{6}	1.31×10^{-7}	5.60×10^{-11}	6.00×10^{-8}
Ethylene oxide	75-21-8	−0.05	−0.3	2.37×10^{5}	1.20×10^{-4}	5.23×10^{-5}	1.48×10^{-4}
Ethylenediamine	107-15-3	−1.62	−2.04	1.00×10^{6}	1.03×10^{-9}	1.77×10^{-10}	1.73×10^{-9}
Ethylenediaminetetraacetic acid	60-00-4	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethylenediaminetetraacetic acid, disodium salt	139-33-3	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethyne	74-86-2	0.5	0.37	1.48×10^{4}	2.40×10^{-2}	2.45×10^{-2}	2.17×10^{-2}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Fatty acids, C18-unsaturated, dimers	61788-89-4	14.6	--	2.31×10^{-10}	4.12×10^{-8}	9.74×10^{-9}	--
FD&C Blue no. 1	3844-45-9	−0.15	--	0.2205	2.25×10^{-35}	--	--
FD&C Yellow no. 5	1934-21-0	−1.82	--	7.388	1.31×10^{-28}	--	--
FD&C Yellow no. 6	2783-94-0	1.4	--	242.7	3.26×10^{-23}	--	--
Formaldehyde	50-00-0	0.35	0.35	5.70×10^{4}	9.29×10^{-5}	6.14×10^{-5}	3.37×10^{-7}
Formamide	75-12-7	−1.61	−1.51	1.00×10^{6}	1.53×10^{-8}	--	1.39×10^{-9}
Formic acid	64-18-6	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Formic acid, potassium salt	590-29-4	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Fumaric acid	110-17-8	0.05	−0.48	1.04×10^{5}	1.35×10^{-12}	8.48×10^{-14}	--
Furfural	98-01-1	0.83	0.41	5.36×10^{4}	1.34×10^{-5}	--	3.77×10^{-6}
Furfuryl alcohol	98-00-0	0.45	0.28	2.21×10^{5}	2.17×10^{-7}	--	7.86×10^{-8}
Galantamine hydrobromide	69353-21-5	2.29	--	1,606	1.70×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Gluconic acid	133-42-6	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--
Glutaraldehyde	111-30-8	−0.18	--	1.67×10^{5}	1.10×10^{-7}	2.39×10^{-8}	--
Glycerol	56-81-5	−1.65	−1.76	1.00×10^{6}	6.35×10^{-9}	1.51×10^{-15}	1.73×10^{-8}
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	135-37-5	−3.04	--	1.90×10^{5}	3.90×10^{-17}	--	--
Glycine, N-(hydroxymethyl)-, monosodium salt	70161-44-3	−3.41	--	7.82×10^{5}	1.80×10^{-12}	--	--
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	5064-31-3	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--
Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)-, trisodium salt	139-89-9	−4.09	--	4.31×10^{5}	3.81×10^{-24}	--	--
Glycolic acid	79-14-1	−1.07	−1.11	1.00×10^{6}	8.54×10^{-8}	6.29×10^{-11}	--
Glycolic acid sodium salt	2836-32-0	−1.07	−1.11	1.00×10^{6}	8.54×10^{-8}	6.29×10^{-11}	--
Glyoxal	107-22-2	−1.66	--	1.00×10^{6}	3.70×10^{-7}	--	3.33×10^{-9}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Glyoxylic acid	298-12-4	−1.4	--	1.00×10^{6}	2.98×10^{-9}	--	--
Heptane	142-82-5	3.78	4.66	3.554	2.27	2.39	2.00
Hexadecyltrimethylammonium bromide	57-09-0	3.18	--	28.77	2.93×10^{-10}	--	--
Hexane	110-54-3	3.29	3.9	17.24	1.71	1.69	1.80
Hexanedioic acid	124-04-9	0.23	0.08	1.67×10^{5}	9.53×10^{-12}	8.10×10^{-13}	4.71×10^{-12}
Hydroxyvalerenic acid	1619-16-5	3.31	--	282.1	--	--	--
Indole	120-72-9	2.05	2.14	1,529	8.86×10^{-7}	1.99×10^{-6}	5.28×10^{-7}
Isoascorbic acid	89-65-6	−1.88	−1.85	1.00×10^{6}	4.07×10^{-8}	--	--
Isobutane	75-28-5	2.23	2.76	175.1	9.69×10^{-1}	1.02	1.19
Isobutene	115-11-7	2.23	2.34	399.2	2.40×10^{-1}	2.34×10^{-1}	2.18×10^{-1}
Isooctanol	26952-21-6	2.73	--	1,379	3.10×10^{-5}	4.66×10^{-5}	9.21×10^{-5}
Isopentyl alcohol	123-51-3	1.26	1.16	4.16×10^{4}	1.33×10^{-5}	1.65×10^{-5}	1.41×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Isopropanol	67-63-0	0.28	0.05	4.02×10^{5}	7.52×10^{-6}	1.14×10^{-5}	8.10×10^{-6}
Isopropanolamine dodecylbenzene	42504-46-1	7.94	8.65	0.001015	1.34×10^{-1}	2.81×10^{-1}	--
Isopropylamine	75-31-0	0.27	0.26	8.38×10^{5}	1.34×10^{-5}	--	4.51×10^{-5}
Isoquinoline	119-65-3	2.14	2.08	1,551	6.88×10^{-7}	4.15×10^{-7}	--
Isoquinoline, reaction products with benzyl chloride and quinoline	68909-80-8	2.14	2.08	1,551	6.88×10^{-7}	4.15×10^{-7}	--
Isoquinolinium, 2-(phenylmethyl)-, chloride	35674-56-7	4.4	--	6.02	1.19×10^{-6}	--	--
Lactic acid	50-21-5	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Lactose	63-42-3	−5.12	--	1.00×10^{6}	4.47×10^{-22}	9.81×10^{-45}	--
Lauryl hydroxysultaine	13197-76-7	−1.3	--	7.71×10^{4}	1.04×10^{-21}	--	--
L-Dilactide	4511-42-6	1.65	--	3,165	1.22×10^{-5}	--	--
L-Glutamic acid	56-86-0	−3.83	−3.69	9.42×10^{5}	1.47×10^{-14}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
L-Lactic acid	79-33-4	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Methane	74-82-8	0.78	1.09	2,610	4.14×10^{-1}	6.58×10^{-1}	6.58×10^{-1}
Methanol	67-56-1	−0.63	−0.77	1.00×10^{6}	4.27×10^{-6}	3.62×10^{-6}	4.55×10^{-6}
Methenamine	100-97-0	−4.15	--	1.00×10^{6}	1.63×10^{-1}	--	1.64×10^{-9}
Methoxyacetic acid	625-45-6	−0.68	--	1.00×10^{6}	4.54×10^{-8}	8.68×10^{-9}	6.42×10^{-9}
Methyl salicylate	119-36-8	2.6	2.55	1,875	4.55×10^{-6}	2.23×10^{-9}	9.81×10^{-5}
Methyl vinyl ketone	78-94-4	0.41	--	6.06×10^{4}	2.61×10^{-5}	1.38×10^{-5}	4.65×10^{-5}
Methylcyclohexane	108-87-2	3.59	3.61	28.4	3.39×10^{-1}	3.30×10^{-1}	4.30×10^{-1}
Methylene bis(thiocyanate)	6317-18-6	0.62	--	2.72×10^{4}	2.61×10^{-8}	--	--
Methylenebis(5-methyloxazolidine)	66204-44-2	−0.58	--	1.00×10^{6}	1.07×10^{-7}	--	--
Morpholine	110-91-8	−0.56	−0.86	1.00×10^{6}	1.14×10^{-7}	3.22×10^{-9}	1.16×10^{-6}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	78-21-7	4.54	--	0.9381	2.66×10^{-12}	--	--
N-(2-Acryloyloxyethyl)-N-benzyl-N,N-dimethylammonium chloride	46830-22-2	−1.39	--	4.42×10^{5}	5.62×10^{-16}	--	--
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	−5.92	--	1.00×10^{6}	1.76×10^{-8}	--	--
N,N,N-Trimethyl-3-((1-oxooctadecyl)amino)-1-propanaminium methyl sulfate	19277-88-4	4.38	--	0.7028	2.28×10^{-16}	--	--
N,N,N-Trimethyloctadecan-1-aminium chloride	112-03-8	4.17	--	2.862	5.16×10^{-10}	--	--
N,N'-Dibutylthiourea	109-46-6	2.57	2.75	2,287	4.17×10^{-6}	--	--
N,N-Dimethyldecylamine oxide	2605-79-0	1.4	--	2,722	4.88×10^{-14}	--	--
N,N-Dimethylformamide	68-12-2	−0.93	−1.01	9.78×10^{5}	7.38×10^{-8}	--	7.39×10^{-8}
N,N-Dimethylmethanamine hydrochloride	593-81-7	0.04	0.16	1.00×10^{6}	3.65×10^{-5}	1.28×10^{-4}	1.04×10^{-4}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
N,N-Dimethyl-methanamine-N-oxide	1184-78-7	−3.02	--	1.00×10^{6}	3.81×10^{-15}	--	--
N,N-dimethyloctadecylamine hydrochloride	1613-17-8	8.39	--	0.008882	4.51×10^{-3}	3.88×10^{-2}	--
N,N'-Methylenebisacrylamide	110-26-9	−1.52	--	7.01×10^{4}	1.14×10^{-9}	--	--
Naphthalene	91-20-3	3.17	3.3	142.1	5.26×10^{-4}	3.70×10^{-4}	4.40×10^{-4}
Naphthalenesulfonic acid, bis(1-methylethyl)-	28757-00-8	2.92	--	43.36	9.29×10^{-10}	--	--
Naphthalenesulphonic acid, bis (1-methylethyl)-methyl derivatives	99811-86-6	4.02	--	3.45	1.13×10^{-9}	--	--
Naphthenic acid ethoxylate	68410-62-8	3.41	--	112.5	3.62×10^{-8}	2.74×10^{-9}	--
Nitrilotriacetamide	4862-18-4	−4.75	--	1.00×10^{6}	1.61×10^{-18}	--	--
Nitrilotriacetic acid	139-13-9	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
N-Methyl-2-pyrrolidone	872-50-4	−0.11	−0.38	2.48×10^{5}	3.16×10^{-8}	--	3.20×10^{-9}
N-Methyldiethanolamine	105-59-9	−1.5	--	1.00×10^{6}	8.61×10^{-11}	2.45×10^{-14}	3.14×10^{-11}
N-Methylethanolamine	109-83-1	−1.15	−0.94	1.00×10^{6}	8.07×10^{-10}	2.50×10^{-10}	--
N-Methyl-N-hydroxyethyl-N-hydroxyethoxyethylamine	68213-98-9	−1.78	--	1.00×10^{6}	1.34×10^{-12}	5.23×10^{-17}	--
N-Oleyl diethanolamide	13127-82-7	6.63	--	0.1268	9.35×10^{-9}	1.94×10^{-12}	--
Oleic acid	112-80-1	7.73	7.64	0.01151	4.48×10^{-5}	1.94×10^{-5}	--
Pentaethylenehexamine	4067-16-7	−3.67	--	1.00×10^{6}	8.36×10^{-24}	2.56×10^{-27}	--
Pentane	109-66-0	2.8	3.39	49.76	1.29	1.20	1.25
Pentyl acetate	628-63-7	2.34	2.3	996.8	5.45×10^{-4}	4.45×10^{-4}	3.88×10^{-4}
Pentyl butyrate	540-18-1	3.32	--	101.9	9.60×10^{-4}	8.88×10^{-4}	--
Peracetic acid	79-21-0	−1.07	--	1.00×10^{6}	1.39×10^{-6}	--	2.14×10^{-6}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Phenanthrene	85-01-8	4.35	4.46	0.677	5.13×10^{-5}	2.56×10^{-5}	4.23×10^{-5}
Phenol	108-95-2	1.51	1.46	2.62×10^{4}	5.61×10^{-7}	6.58×10^{-7}	3.33×10^{-7}
Phosphonic acid (dimethylamino(methylene))	29712-30-9	−1.9	--	1.00×10^{6}	1.00×10^{-24}	--	--
Phosphonic acid, (((2-[(2-hydroxyethyl)(phosphonomethyl)amino)ethyl)imino]bis(methylene))bis-, compd. with 2-aminoethanol	129828-36-0	−6.73	--	1.00×10^{6}	5.29×10^{-42}	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, potassium salt	67953-76-8	−0.01	--	1.34×10^{5}	9.79×10^{-26}	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, tetrasodium salt	3794-83-0	−0.01	--	1.34×10^{5}	9.79×10^{-26}	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-	15827-60-8	−9.72	--	1.00×10^{6}	--	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-, ammonium salt (1:x)	70714-66-8	−9.72	--	1.00×10^6	--	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-, sodium salt	22042-96-2	−9.72	--	1.00×10^6	--	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[6,1-hexanediylnitrilobis (methylene)]]tetrakis-	34690-00-1	−5.79	--	1.00×10^6	--	--	--
Phthalic anhydride	85-44-9	2.07	1.6	3,326	6.35×10^{-6}	--	1.63×10^{-8}
Poly(oxy-1,2-ethanediyl), .alpha.-(octylphenyl)-.omega.-hydroxy-, branched	68987-90-6	5.01	--	3.998	1.24×10^{-7}	1.07×10^{-6}	--
Potassium acetate	127-08-2	0.09	−0.17	4.76×10^5	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Potassium oleate	143-18-0	7.73	7.64	0.01151	4.48×10^{-5}	1.94×10^{-5}	--
Propane	74-98-6	1.81	2.36	368.9	7.30×10^{-1}	6.00×10^{-1}	7.07×10^{-1}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Propanol, 1(or 2)-(2-methoxymethylethoxy)-	34590-94-8	−0.27	--	4.27×10^{5}	1.15×10^{-9}	1.69×10^{-9}	--
Propargyl alcohol	107-19-7	−0.42	−0.38	9.36×10^{5}	5.88×10^{-7}	--	1.15×10^{-6}
Propylene carbonate	108-32-7	0.08	−0.41	2.58×10^{5}	3.63×10^{-4}	--	3.45×10^{-8}
Propylene pentamer	15220-87-8	6.28	--	0.05601	3.92×10^{-1}	1.09×10^{-3}	--
p-Xylene	106-42-3	3.09	3.15	228.6	6.56×10^{-3}	6.14×10^{-3}	6.90×10^{-3}
Pyrimidine	289-95-2	−0.06	−0.4	2.87×10^{5}	2.92×10^{-6}	--	--
Pyrrole	109-97-7	0.88	0.75	3.12×10^{4}	9.07×10^{-6}	7.73×10^{-6}	1.80×10^{-5}
Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides	68424-95-3	2.69	--	90.87	2.20×10^{-10}	--	--
Quinaldine	91-63-4	2.69	2.59	498.5	7.60×10^{-7}	2.13×10^{-6}	--
Quinoline	91-22-5	2.14	2.03	1,711	6.88×10^{-7}	1.54×10^{-6}	1.67×10^{-6}
Rhodamine B	81-88-9	6.03	--	0.0116	--	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium 1-octanesulfonate	5324-84-5	1.06	--	5,864	9.15×10^{-8}	--	--
Sodium 2-mercaptobenzothiolate	2492-26-4	2.86	2.42	543.4	3.63×10^{-8}	--	--
Sodium acetate	127-09-3	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Sodium benzoate	532-32-1	1.87	1.87	2,493	1.08×10^{-7}	4.55×10^{-8}	3.81×10^{-8}
Sodium bicarbonate	144-55-8	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium bis(tridecyl) sulfobutanedioate	2673-22-5	11.15	--	7.46×10^{-9}	8.51×10^{-11}	--	--
Sodium C14-16 alpha-olefin sulfonate	68439-57-6	4.36	--	2.651	4.95×10^{-7}	--	--
Sodium caprylamphopropionate	68610-44-6	−0.26	--	615.1	1.19×10^{-9}	2.45×10^{-10}	--
Sodium carbonate	497-19-8	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium chloroacetate	3926-62-3	0.34	0.22	1.95×10^{5}	1.93×10^{-7}	8.88×10^{-8}	9.26×10^{-9}
Sodium decyl sulfate	142-87-0	1.44	--	1,617	1.04×10^{-7}	--	--
Sodium D-gluconate	527-07-1	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium diacetate	126-96-5	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Sodium dichloroisocyanurate	2893-78-9	1.28	--	3,613	3.22×10^{-12}	--	--
Sodium dl-lactate	72-17-3	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Sodium dodecyl sulfate	151-21-3	2.42	--	163.7	1.84×10^{-7}	--	--
Sodium erythorbate (1:1)	6381-77-7	−1.88	−1.85	1.00×10^{6}	4.07×10^{-8}	--	--
Sodium ethasulfate	126-92-1	0.38	--	1.82×10^{4}	5.91×10^{-8}	--	--
Sodium formate	141-53-7	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Sodium hydroxymethanesulfonate	870-72-4	−3.85	--	1.00×10^{6}	4.60×10^{-13}	--	--
Sodium l-lactate	867-56-1	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Sodium maleate (1:x)	18016-19-8	0.05	−0.48	1.04×10^{5}	1.35×10^{-12}	8.48×10^{-14}	--
Sodium N-methyl-N-oleoyltaurate	137-20-2	4.43	--	0.4748	1.00×10^{-12}	--	--
Sodium octyl sulfate	142-31-4	0.46	--	1.58×10^{4}	5.91×10^{-8}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium salicylate	54-21-7	2.24	2.26	3,808	1.42×10^{-8}	5.60×10^{-12}	7.34×10^{-9}
Sodium sesquicarbonate	533-96-0	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium thiocyanate	540-72-7	0.58	--	4.36×10^{4}	1.46×10^{-4}	--	--
Sodium trichloroacetate	650-51-1	1.44	1.33	1.20×10^{4}	2.39×10^{-8}	--	1.35×10^{-8}
Sodium xylenesulfonate	1300-72-7	−0.07	--	5.89×10^{4}	3.06×10^{-9}	--	--
Sorbic acid	110-44-1	1.62	1.33	1.94×10^{4}	5.72×10^{-7}	4.99×10^{-8}	--
Sorbitan sesquioleate	8007-43-0	14.32	--	2.31×10^{-11}	7.55×10^{-12}	1.25×10^{-16}	--
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	5.89	--	0.01914	1.42×10^{-12}	5.87×10^{-20}	--
Sorbitan, monooctadecanoate	1338-41-6	6.1	--	0.01218	1.61×10^{-12}	2.23×10^{-19}	--
Sorbitan, tri-(9Z)-9-octadecenoate	26266-58-0	22.56	--	1.12×10^{-19}	4.02×10^{-11}	2.68×10^{-13}	--
Styrene	100-42-5	2.89	2.95	343.7	2.76×10^{-3}	2.81×10^{-3}	2.75×10^{-3}
Sucrose	57-50-1	−4.27	−3.7	1.00×10^{6}	4.47×10^{-22}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sulfan blue	129-17-9	−1.34	--	50.67	1.31×10^{-26}	--	--
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	68955-19-1	3.9	--	5.165	4.29×10^{-7}	--	--
Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	68187-17-7	0.46	--	1.58×10^{4}	5.91×10^{-8}	--	--
Symclosene	87-90-1	0.94	--	4,610	6.19×10^{-11}	--	--
tert-Butyl hydroperoxide	75-91-2	0.94	--	1.97×10^{4}	1.60×10^{-5}	--	--
tert-Butyl perbenzoate	614-45-9	2.89	--	159.2	2.06×10^{-4}	--	--
Tetradecane	629-59-4	7.22	7.2	0.009192	1.65×10^{1}	2.68×10^{1}	9.20
Tetradecyldimethylbenzylammonium chloride	139-08-2	3.91	--	3.608	1.34×10^{-11}	--	--
Tetraethylene glycol	112-60-7	−2.02	--	1.00×10^{6}	4.91×10^{-13}	5.48×10^{-19}	--
Tetraethylenepentamine	112-57-2	−3.16	--	1.00×10^{6}	2.79×10^{-20}	4.15×10^{-23}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	−5.03	--	1.00×10^{6}	9.17×10^{-13}	--	--
Tetramethylammonium chloride	75-57-0	−4.18	--	1.00×10^{6}	4.17×10^{-12}	--	--
Thiamine hydrochloride	67-03-8	0.95	--	3,018	8.24×10^{-17}	--	--
Thiocyanic acid, ammonium salt	1762-95-4	0.58	--	4.36×10^{4}	1.46×10^{-4}	--	--
Thioglycolic acid	68-11-1	0.03	0.09	2.56×10^{5}	1.94×10^{-8}	--	--
Thiourea	62-56-6	−1.31	−1.08	5.54×10^{5}	1.58×10^{-7}	--	1.98×10^{-9}
Toluene	108-88-3	2.54	2.73	573.1	5.95×10^{-3}	5.73×10^{-3}	6.64×10^{-3}
Tributyl phosphate	126-73-8	3.82	4	7.355	3.19×10^{-6}	--	1.41×10^{-6}
Tributyltetradecylphosphonium chloride	81741-28-8	11.22	--	7.90×10^{-7}	2.61×10^{-1}	--	--
Tridecane	629-50-5	6.73	--	0.02746	1.24×10^{1}	1.90×10^{1}	2.88
Triethanolamine	102-71-6	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Triethanolamine hydrochloride	637-39-8	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}
Triethanolamine hydroxyacetate	68299-02-5	−2.97	--	1.00×10^{6}	6.28×10^{-11}	--	--
Triethyl citrate	77-93-0	0.33	--	2.82×10^{4}	6.39×10^{-10}	--	3.84×10^{-9}
Triethyl phosphate	78-40-0	0.87	0.8	1.12×10^{4}	5.83×10^{-7}	--	3.60×10^{-8}
Triethylene glycol	112-27-6	−1.75	−1.75	1.00×10^{6}	3.16×10^{-11}	2.56×10^{-16}	--
Triethylenetetramine	112-24-3	−2.65	--	1.00×10^{6}	9.30×10^{-17}	6.74×10^{-19}	--
Triisopropanolamine	122-20-3	−1.22	--	1.00×10^{6}	9.77×10^{-12}	4.35×10^{-18}	--
Trimethanolamine	14002-32-5	−3.95	--	1.00×10^{6}	1.42×10^{-8}	--	--
Trimethylamine	75-50-3	0.04	0.16	1.00×10^{6}	3.65×10^{-5}	1.28×10^{-4}	1.04×10^{-4}
Tripotassium citrate monohydrate	6100-05-6	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Tripropylene glycol monomethyl ether	25498-49-1	−0.2	--	1.96×10^{5}	2.36×10^{-11}	4.55×10^{-13}	--
Trisodium citrate	68-04-2	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Trisodium citrate dihydrate	6132-04-3	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Trisodium ethylenediaminetetraacetate	150-38-9	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Trisodium ethylenediaminetriacetate	19019-43-3	−4.32	--	1.00×10^{6}	3.58×10^{-20}	--	--
Tromethamine	77-86-1	−1.56	--	1.00×10^{6}	8.67×10^{-13}	--	--
Undecane	1120-21-4	5.74	--	0.2571	7.04	9.52	1.93
Urea	57-13-6	−1.56	−2.11	4.26×10^{5}	3.65×10^{-10}	--	1.74×10^{-12}
Xylenes	1330-20-7	3.09	3.2	207.2	6.56×10^{-3}	6.14×10^{-3}	7.18×10^{-3}

"--" indicates no information available.

The EPI (Estimation Programs Interface) Suite™ (U.S. EPA, 2012a) is an open-source, Windows®-based suite of physicochemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation. More information on EPI Suite™ is available at http://www.epa.gov/oppt/exposure/pubs/episuite.htm.

Although only physicochemical properties from EPI Suite™ are provided here, other sources of information were also consulted. QikProp (Schrodinger, 2012) and LeadScope® (Inc., 2012) are commercial products designed primarily as drug development and screening tools. QikProp is specifically focused on drug discovery and provides predictions for physically significant descriptors and pharmaceutically (and toxicologically) relevant properties useful in predicting ADME (adsorption, distribution, metabolism, and excretion) characteristics of drug candidates. QikProp's use of whole-molecule descriptors that have a straightforward physical interpretation (as opposed to fragment-based descriptors).

LeadScope® is a program designed for interpreting chemical and biological screening data that can assist pharmaceutical scientists in finding promising drug candidates. The software organizes the chemical data by structural features familiar to medicinal chemists. Graphs are used to summarize the data, and structural classes are highlighted that are statistically correlated with biological activity. It incorporates chemically-based data mining, visualization, and advanced informatics techniques (e.g., prediction tools, scaffold generators). Note that properties generated by QikProp and LeadScope® are generally more relevant to drug development than to environmental assessment.

Physicochemical properties of chemicals were generated from the two-dimensional (2-D) chemical structures from the EPA National Center for Computational Toxicology's Distributed Structure-Searchable Toxicity (NCCT DSSTox) Database Network in structure-data file (SDF) format. For EPI Suite™ properties, both the desalted and non-desalted 2-D files were run using the program's batch mode (i.e., processing many molecules at once) to calculate environmentally-relevant, chemical property descriptors. The chemical descriptors in QikProp require 3-D chemical structures. For these calculations, the 2-D desalted chemical structures were converted to 3-D using the Rebuild3D function in the Molecular Operating Environment software (CCG, 2011). All computed physicochemical properties are added into the structure-data file prior to assigning toxicological properties.

Both LeadScope® and Qikprop software require input of desalted structures. Therefore, the structures were desalted, a process where salts and complexes are simplified to the neutral, uncomplexed form of the chemical, using "Desalt Batch" option in ACD Labs ChemFolder. All LeadScope® general chemical descriptors (Parent Molecular Weight, AlogP, Hydrogen Bond Acceptors**,** Hydrogen Bond Donors, Lipinski Score, Molecular Weight, Parent Atom Count, Polar Surface Area, and Rotatable Bonds) were calculated by default.

All physicochemical properties generated from EPI Suite™, QikProp, and LeadScope® will be made available to the public in an electronic format in 2015.

C.2. References for Appendix C

Afzal, W; Mohammadi, AH; Richon, D. (2009). Volumetric properties of mono-, di-, tri-, and polyethylene glycol aqueous solutions from (273.15 to 363.15) K: experimental measurements and correlations. Journal of Chemical and Engineering Data 54: 1254-1261. http://dx.doi.org/10.1021/je800694a

Alfa Aesar. (2015). A16163: Formaldehyde, 37% w/w aq. soln., stab. with 7-8% methanol. Available online at https://www.alfa.com/en/catalog/A16163 (accessed May 4, 2015).

Baragi, JG; Maganur, S; Malode, V; Baragi, SJ. (2013). Excess molar volumes and refractive indices of binary liquid mixtures of acetyl acetone with n-Nonane, n-Decane and n-Dodecane at (298.15, 303.15, and 308.15) K. Journal of Molecular Liquids 178: 175-177. http://dx.doi.org/10.1016/j.molliq.2012.11.022

Bennett, GM; Yuill, JL. (1935). The crystal form of anhydrous citric acid. J Chem Soc 1935: 130. http://dx.doi.org/10.1039/JR9350000130

Biilmann, E. (1906). [Studien über organische Thiosäuren III]. Justus Liebigs Annalen der Chemie 348: 133-143. http://dx.doi.org/10.1002/jlac.19063480110

Biltz, W; Balz, G. (1928). [Über molekular- und atomvolumina. XVIII. Das volumen des ammoniaks in kristallisierten ammoniumsalzen]. Zeitschrift für Anorganische und Allgemeine Chemie 170: 327-341. http://dx.doi.org/10.1002/zaac.19281700141

Blanco, A; Garcia-Abuin, A; Gomez-Diaz, D; Navaza, JM; Villaverde, OL. (2013). Density, speed of sound, viscosity, surface tension, and excess volume of n-ethyl-2-pyrrolidone plus ethanolamine (or diethanolamine or triethanolamine) from T = (293.15 to 323.15) K. Journal of Chemical and Engineering Data 58: 653-659. http://dx.doi.org/10.1021/je301123j

Carpenter, EL; Davis, HS. (1957). Acrylamide. Its preparation and properties. Journal of Applied Chemistry 7: 671-676. http://dx.doi.org/10.1002/jctb.5010071206

Casanova, C; Wilhelm, E; Grolier, JPE; Kehiaian, HV. (1981). Excess volumes and excess heat-capacities of (water + alkanoic acid). The Journal of Chemical Thermodynamics 13: 241-248. http://dx.doi.org/10.1016/0021-9614(81)90123-3

CCG (Chemical Computing Group). (2011). Molecular Operating Environment (MOE) Linux (Version 2011.10) [Computer Program]. Montreal, Quebec. Retrieved from http://www.chemcomp.com/software.htm

Chafer, A; Lladosa, E; Monton, JB; Cruz Burguet, M, a. (2010). Liquid-liquid equilibria for the system 1-methyl propyl ethanoate (1) + acetic acid (2) + water (3) at (283.15 and 323.15) K. Journal of Chemical and Engineering Data 55: 523-525. http://dx.doi.org/10.1021/je900332x

Chasib, KF. (2013). Extraction of phenolic pollutants (phenol and p-chlorophenol) from industrial wastewater. Journal of Chemical and Engineering Data 58: 1549-1564. http://dx.doi.org/10.1021/je4001284

de Oliveira, LH; da Silva, JL, Jr; Aznar, M. (2011). Apparent and partial molar volumes at infinite dilution and solid-liquid equilibria of dibenzothiophene plus alkane systems. Journal of Chemical and Engineering Data 56: 3955-3962. http://dx.doi.org/10.1021/je200327s

Dejoye Tanzi, C; Abert Vian, M; Ginies, C; Elmaataoui, M; Chemat, F. (2012). Terpenes as green solvents for extraction of oil from microalgae. Molecules 17: 8196-8205. http://dx.doi.org/10.3390/molecules17078196

Dhondge, SS; Pandhurnekar, CP; Parwate, DV. (2010). Density, speed of sound, and refractive index of aqueous binary mixtures of some glycol ethers at T=298.15 K. Journal of Chemical and Engineering Data 55: 3962-3968. http://dx.doi.org/10.1021/je901072c

Dubey, GP; Kumar, K. (2011). Thermodynamic properties of binary liquid mixtures of diethylenetriamine with alcohols at different temperatures. Thermochim Acta 524: 7-17. http://dx.doi.org/10.1016/j.tca.2011.06.003

Dubey, GP; Kumar, K. (2013). Studies of thermodynamic, thermophysical and partial molar properties of liquid mixtures of diethylenetriamine with alcohols at 293.15 to 313.15 K. Journal of Molecular Liquids 180: 164-171. http://dx.doi.org/10.1016/j.molliq.2013.01.011

Dyshin, AA; Eliseeva, OV; Kiselev, MG; Al'per, GA. (2008). The volume characteristics of solution of naphthalene in heptane-ethanol mixtures at 298.15 K. Russian Journal of Physical Chemistry A, Focus on Chemistry 82: 1258-1261. http://dx.doi.org/10.1134/S0036024408080037

Egorov, GI; Makarov, DM; Kolker, AM. (2013). Volume properties of liquid mixture of water plus glycerol over the temperature range from 278.15 to 348.15 K at atmospheric pressure. Thermochim Acta 570: 16-26. http://dx.doi.org/10.1016/j.tca.2013.07.012

Fadeeva, YA; Shmukler, LE; Safonova, LP. (2004). Physicochemical properties of the H3PO4-dimethylformamide system. Russian Journal of General Chemistry 74: 174-178. http://dx.doi.org/10.1023/B:RUGC.0000025496.07304.66

Faria, MAF; Martins, RJ; Cardoso, MJE, M; Barcia, OE. (2013). Density and viscosity of the binary systems ethanol + butan-1-ol, + pentan-1-ol, + heptan-1-ol, + octan-1-ol, nonan-1-ol, + decan-1-ol at 0.1 mpa and temperatures from 283.15 K to 313.15 K. Journal of Chemical and Engineering Data 58: 3405-3419. http://dx.doi.org/10.1021/je400630f

Fels, G. (1900). Ueber die Frage der isomorphen vertretung von halogen und hydroxyl. In Zeitschrift fur Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie. Frankfurt: Leipzig. http://babel.hathitrust.org/cgi/pt?id=uc1.b3327977;view=1up;seq=5

finemech (finemech Precision Mechanical Components). (2012). Technical resources: Liquid nitrogen, LN2. Available online at http://www.finemech.com/tech_resources/liquid_nitrogen.html

Fuess, H; Bats, JW; Dannohl, H; Meyer, H; Schweig, A. (1982). Comparison of observed and calculated densities. XII. Deformation density in complex anions. II. Experimental and theoretical densities in sodium formate. Acta Crystallogr B B38: 736-743. http://dx.doi.org/10.1107/S0567740882003999

Fujino, S; Hwang, C; Morinaga, K. (2004). Density, surface tension, and viscosity of PbO-B2O3-SiO2 glass melts. Journal of the American Ceramic Society 87: 10-16. http://dx.doi.org/10.1111/j.1151-2916.2004.tb19937.x

Hagen, R; Kaatze, U. (2004). Conformational kinetics of disaccharides in aqueous solutions. J Chem Phys 120: 9656-9664. http://dx.doi.org/10.1063/1.1701835

Harlow, A; Wiegand, G; Franck, EU. (1997). The Density of Ammonia at High Pressures to 723 K and 950 MPa. 101: 1461-1465. http://dx.doi.org/10.1002/bbpc.199700007

Haynes, WM. (2014). CRC handbook of chemistry and physics. In WM Haynes (Ed.), (95 ed.). Boca Raton, FL: CRC Press. http://www.hbcpnetbase.com/

He, YM; Jiang, RF; Zhu, F; Luan, TG; Huang, ZQ; Ouyang, GF. (2008). Excess molar volumes and surface tensions of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with isopropyl acetate and isobutyl acetate at (298.15, 308.15, and 313.15)K. Journal of Chemical and Engineering Data 53: 1186-1191. http://dx.doi.org/10.1021/je800046k

Huffman, HM; Fox, SW. (1938). Thermal data. X. The heats of combustion and free energies, at 25, of some organic compounds concerned in carbohydrate metabolism. J Am Chem Soc 60: 1400-1403. http://dx.doi.org/10.1021/ja01273a036

Inc., L. (2012). Leadscope [Computer Program]. Columbus, Ohio. Retrieved from http://www.leadscope.com

IUPAC (International Union of Pure and Applied Chemistry). (2014). Global availability of information on agrochemicals: Triisopropanolamine. Available online at http://sitem.herts.ac.uk/aeru/iupac/Reports/1338.htm

Kiselev, VD; Kashaeva, HA; Shakirova, II; Potapova, LN; Konovalov, AI. (2012). Solvent effect on the enthalpy of solution and partial molar volume of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate. Journal of Solution Chemistry 41: 1375-1387. http://dx.doi.org/10.1007/s10953-012-9881-9

Krakowiak, J; Bobicz, D; Grzybkowski, W. (2001). Limiting partial molar volumes of tetra-n-alkylammonium perchlorates in N,N-dimethylacetamide, triethylphosphate and dimethyl sulfoxide at T=298.15 K. The Journal of Chemical Thermodynamics 33: 121-133. http://dx.doi.org/10.1006/jcht.2000.0725

Laavi, H; Pokki, JP; Uusi-Kyyny, P; Massimi, A; Kim, Y; Sapei, E; Alopaeus, V. (2013). Vapor-liquid equilibrium at 350 k, excess molar enthalpies at 298 K, and excess molar volumes at 298 K of binary mixtures containing ethyl acetate, butyl acetate, and 2-butanol. Journal of Chemical and Engineering Data 58: 1011-1019. http://dx.doi.org/10.1021/je400036b

Laavi, H; Zaitseva, A; Pokki, JP; Uusi-Kyyny, P; Kim, Y; Alopaeus, V. (2012). Vapor-liquid equilibrium, excess molar enthalpies, and excess molar volumes of binary mixtures containing methyl isobutyl ketone (MIBK) and 2-butanol, tert-pentanol, or 2-ethyl-1-hexanol. Journal of Chemical and Engineering Data 57: 3092-3101. http://dx.doi.org/10.1021/je300678r

Mak, TCW. (1965). Hexamethylenetetramine hexahydrate: A new type of clathrate hydrate. J Chem Phys 43: 2799. http://dx.doi.org/10.1063/1.1697212

Martinez-Reina, M; Amado-Gonzalez, E; Mauricio Munoz-Munoz, Y. (2012). Study of liquid-liquid equilibria of toluene plus (hexane, heptane, or cyclohexane) with 1-ethyl-3-methylimidazolium ethylsulfate at 308.15 K. Bull Chem Soc Jpn 85: 1138-1144. http://dx.doi.org/10.1246/bcsj.20120112

Masood, AKM; Pethrick, RA; Swinton, FL. (1976). Physicochemical studies of super-cooled liquids - cyclic carbonates and alpha,beta-unsaturated aldehydes. Faraday Trans 1 72: 20-28. http://dx.doi.org/10.1039/f19767200020

Moosavi, M; Motahari, A; Omrani, A; Rostami, AA. (2013). Thermodynamic study on some alkanediol solutions: Measurement and modeling. Thermochim Acta 561: 1-13. http://dx.doi.org/10.1016/j.tca.2013.03.010

Oka, S. (1962). Studies on lactone formation in vapor phase. III. Mechanism of lactone formation from diols. Bull Chem Soc Jpn 35: 986-989. http://dx.doi.org/10.1246/bcsj.35.986

Pal, A; Kumar, H; Maan, R; Sharma, HK. (2013). Densities and speeds of sound of binary liquid mixtures of some n-alkoxypropanols with methyl acetate, ethyl acetate, and n-butyl acetate at T = (288.15, 293.15, 298.15, 303.15, and 308.15) K. Journal of Chemical and Engineering Data 58: 225-239. http://dx.doi.org/10.1021/je300789a

Pijper, WP. (1971). Molecular and crystal structure of glycollic acid. Acta Crystallogr B B27: 344-348. http://dx.doi.org/10.1107/S056774087100219X

Radwan, MHS; Hanna, AA. (1976). Binary azeotropes containing butyric acids. Journal of Chemical and Engineering Data 21: 285-289. http://dx.doi.org/10.1021/je60070a032

Rani, M; Maken, S. (2013). Excess molar enthalpies and excess molar volumes of formamide+1-propanol or 2-propanol and thermodynamic modeling by Prigogine-Flory-Patterson theory and Treszczanowicz-Benson association model. Thermochim Acta 559: 98-106. http://dx.doi.org/10.1016/j.tca.2013.02.010

Rawat, BS; Gulati, IB; Mallik, KL. (1976). Study of some sulphur-group solvents for aromatics extraction by gas chromatography. Journal of Applied Chemistry and Biotechnology 26: 247-252. http://dx.doi.org/10.1002/jctb.5020260504

Rodnikova, MN; Solonina, IA; Egorov, GI; Makarov, DM; Gunina, MA. (2012). The bulk properties of dioxane solutions in ethylene glycol at 2575C. Russian Journal of Physical Chemistry A, Focus on Chemistry 86: 330-332. http://dx.doi.org/10.1134/S0036024412020239

Sarkar, BK; Choudhury, A; Sinha, B. (2012). Excess molar volumes, excess viscosities and ultrasonic speeds of sound of binary mixtures of 1,2-dimethoxyethane with some aromatic liquids at 298.15 K. Journal of Solution Chemistry 41: 53-74. http://dx.doi.org/10.1007/s10953-011-9780-5

Sarkar, L; Roy, MN. (2009). Density, viscosity, refractive index, and ultrasonic speed of binary mixtures of 1,3-dioxolane with 2-methoxyethanol, 2-ethoxyethanol, 2-butoxyethanol, 2-propylamine, and cyclohexylamine. Journal of Chemical and Engineering Data 54: 3307-3312. http://dx.doi.org/10.1021/je900240s

Schrodinger. (2012). Qikprop [Computer Program]. New York, New York: Schrodinger, LLC. Retrieved from http://www.schrodinger.com/products/14/17

Shanley, P; Collin, RL. (1961). The crystal structure of the high temperature form of choline chloride. Acta Cryst 14: 79-80. http://dx.doi.org/10.1107/S0365110X61000292

Sigma-Aldrich. (2007). Material safety data sheet: Tert-butyl hydroperoxide (70% solution in water). Available online at http://www.orcbs.msu.edu/msds/111607_DLI_027_TERT-BUTYL.PDF

Sigma-Aldrich. (2010). Product information: Sodium chloride. Available online at https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Sigma-Aldrich/Product_Information_Sheet/s7653pis.pdf

Sigma-Aldrich. (2014a). Material safety data sheet: Phosphorus acid. Available online at http://www.sigmaaldrich.com/catalog/product/sial/215112?lang=en&region=US

Sigma-Aldrich. (2014b). Material safety data sheet: Potassium carbonate. Available online at http://www.sigmaaldrich.com/catalog/product/aldrich/367877?lang=en&region=US

Sigma-Aldrich. (2015a). Material safety data sheet: Aluminum chloride [Fact Sheet]. St. Louis, MO. http://www.sigmaaldrich.com/catalog/product/aldrich/563919?lang=en&region=US

Sigma-Aldrich. (2015b). Material safety data sheet: Peracetic acid solution. Available online at http://www.sigmaaldrich.com/catalog/product/sial/269336?lang=en&region=US

Sigma-Aldrich. (2015c). Material safety data sheet: Sulfur dioxide. Available online at http://www.sigmaaldrich.com/catalog/product/aldrich/295698?lang=en&region=US

Sigma-Aldrich. (2015d). Material safety data sheet: Sulfuric acid. Available online at http://www.sigmaaldrich.com/catalog/product/aldrich/339741?lang=en&region=US

Sigma-Aldrich. (2015e). Material safety data sheet: Trimethyl borate. Available online at http://www.sigmaaldrich.com/catalog/product/aldrich/447218?lang=en&region=US

Smirnov, VI; Badelin, VG. (2013). Enthalpy characteristics of dissolution of L-tryptophan in water plus formamides binary solvents at 298.15 K. Russian Journal of Physical Chemistry A, Focus on Chemistry 87: 1165-1169. http://dx.doi.org/10.1134/S0036024413070285

Steinhauser, O; Boresch, S; Bertagnolli, H. (1990). The effect of density variation on the structure of liquid hydrogen chloride. A Monte Carlo study. J Chem Phys 93: 2357-2363. http://dx.doi.org/10.1063/1.459015

Thalladi, VR; Nusse, M; Boese, R. (2000). The melting point alternation in alpha,omega-alkanedicarboxylic acids. J Am Chem Soc 122: 9227-9236. http://dx.doi.org/10.1021/ja0011459

U.S. EPA (U.S. Environmental Protection Agency). (2012a). Estimation Programs Interface Suite for Microsoft Windows (EPI Suite) [Computer Program]. Washington DC: US Environmental Protection Agency. Retrieved from http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

U.S. EPA (U.S. Environmental Protection Agency). (2015c). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0: Project database [EPA Report]. (EPA/601/R-14/003). Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development. http://www2.epa.gov/hfstudy/epa-project-database-developed-fracfocus-1-disclosures

Vijaya Kumar, R; Anand Rao, M; Venkateshwara Rao, M; Ravi Kumar, YVL; Prasad, DHL. (1996). Bubble temperature measurements on 2-propyn-1-ol with 1,2-dichloroethane, 1,1,1-trichloroethane, and 1,1,2,2-tetrachloroethane. Journal of Chemical and Engineering Data 41: 1020-1023. http://dx.doi.org/10.1021/je9600156

Wilt, JW. (1956). Notes - the halodecarboxylation of cyanoacetic acid. J Org Chem 21: 920-921. http://dx.doi.org/10.1021/jo01114a607

Xiao, LN; Xu, JN; Hu, YY; Wang, LM; Wang, Y; Ding, H; Cui, XB; Xu, JQ. (2013). Synthesis and characterizations of the first [V16O39Cl]6- (V16O39) polyanion. Dalton Transactions (Online) 42: 5247-5251. http://dx.doi.org/10.1039/c3dt33081h

Zhang, L; Guo, Y; Xiao, J; Gong, X; Fang, W. (2011). Density, refractive index, viscosity, and surface tension of binary mixtures of exo-tetrahydrodicyclopentadiene with some n-alkanes from (293.15 to 313.15) K. Journal of Chemical and Engineering Data 56: 4268-4273. http://dx.doi.org/10.1021/je200757a

Zhang, Z; Yang, L; Xing, Y; Li, W. (2013). Vapor-liquid equilibrium for ternary and binary mixtures of 2-isopropoxypropane, 2-propanol, and n,n-dimethylacetamide at 101.3 kPa. Journal of Chemical and Engineering Data 58: 357-363. http://dx.doi.org/10.1021/je300994y