Section 2

Alcohols

Methanol

Alternative names
Methyl alcohol, wood alcohol, carbinol, **not** methylated spirit

Reference codes			
CAS number	67 56 1	Hazchem code	2PE
UN number	1230	EPA code	U154
Physical properties			
Molecular weight	32	Cubic expansion coeff (per °C × 10^3)	1.2
Empirical formula	$C_1H_4O_1$	Surface tension (@20°C dyn/cm)	22.6
Boiling point (°C)	64	Absolute viscosity (@25°C cP)	0.6
Freezing point (°C)	–98	Refractive index (25°C)	1.326
Specific gravity (20/4)	0.792		
Fire hazards			
Flash point (closed cup °C)	15	Lower explosive limit (ppm)	60000
Autoignition temperature (°C)	470	Upper explosive limit (ppm)	365000
Electrical conductivity	1.5E–9		
Health hazards			
IDLH (ppm)	25000	Vapour concentration @21°C ppm	156000
OES-TWA	200	Vapour density (relative to air)	1.11
OES-STEL	250	Vapour pressure @21°C mmHg	103
Odour threshold (ppm)	6000	POCP	12.3
Aqueous effluent			
Solubility in water (25°C %w/w)		Total	
Solubility of water in (25°C %w/w)		Total	
Log_{10} activated carbon partition		0.86	
Log_{10} partition in octanol/water (w/w)		–0.82	
Biological oxygen demand w/w (days)		1.12 (5)	
Theoretical oxygen demand w/w		1.5	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	8.08097	
	B	1582.271	
	C	239.726	
Cox chart	A	8.23606	
	B	1579.9	
Solvent properties			
Solubility parameter	14.5	Kauri butanol value	380
Dipole (D)	1.7	Evaporation time (ether = 1)	6.3
Dielectric constant (20°C)	32.6	Evaporation time (BuAc = 1)	4.1
Polarity (water 100)	76.2		
Thermal information			
Latent heat (cal/mol)	8426		
Nett heat of combustion (kcal/gmol)	150		
Specific heat (cal/mol/°C)	19.5		
Critical pressure (MN/m^2)	7.96		
Critical temperature (K)	513		
Latent heat of fusion (cal/mol)	758		
Van der Waals' volume	1.43		
Van der Waals' surface area	1.43		
Molar volume	40.4		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	8	31	2055	11.2	2e/132		
n-Hexane	50	68	2087	16.0	2a/253		
n-Heptane	52	59	2101	22.1	2c/243		
n-Octane	72	63	2113	45.1	2c/249		
n-Nonane	83	64	2120	38.6	2e/191		
n-Decane	None		2126	49.7	2e/193		
2,2,4-TMP	53	59	2114	28.1	2c/250		
Cyclohexane	38	54	2079	18.3	2a/239		
Benzene	39	58	2066	7.4	2a/205		
Toluene	69	64	2098	8.4	2a/268		
Ethylbenzene	None		2106	10.3	2c/245		
Xylenes	None		2108	10.3	2c/247		
C_9 Aromatics	None		2116				
Tetralin							
Alcohols							
Methanol	–		–	–	–	–	–
Ethanol	None		1944	1.0	2a/50		
n-Propanol	None			1.3	2a/122		
i-Propanol	None		1978a	0.9	2a/123		
n-Butanol	None		2015	1.3	2a/169		
i-Butanol	None			1.3	2a/171		
s-Butanol				0.7	2c/128		
n-Amyl alc.	None		2056	1.4	2a/202		
i-Amyl alc.	None			1.4	2a/201		
Cyclohexanol							
1-Octanol							
Ethanediol	None		1945		2a/62		
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	None		1979		2c/98		
EEE							
EGBE							
Chlorinated							
MDC	93	38	1544	2.1	2a/24		
Chloroform	87	38	1430	2.7	2a/23		
Carbon tet.	79	56	1090	7.0	2a/1		
1,2-EDC	32	61	1930	5.4	2a/44		
1,1,1-TCA	22	56	1923				
TCE	38	59	1915	8.3	2a/40		
Perk.	64	64	1914	17.9	2a/37		
MCB	None		2063	7.8	2a/204		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	12	56	1963	1.8	2a/68		
MEK	70	64	1993	2.1	2a/133		
MIBK	None		2084	3.3	2a/248		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	98	62		3.2	2a/170		
DIPE	24	57	2091a	4.3	2a/261		
Dibutyl ether				10.6			
MTBE	10	51	2058	3.1	2c/160		
1,4-Dioxane	None		1998	2.2	2a/148		
THF	31	59	1996	2.2	2a/141		
Esters							
Me acetate	19	54	1967	2.9	2a/92		
Et acetate	46	62	1999	2.8	2a/154		
i-Propyl acetate	80	65	2046				
n-Butyl acetate				5.8	2c/213		
Cellosolve acetate							
Miscellaneous							
DMF	None			0.8	2a/115		
DMAc							
DMSO				0.25	2c/62		
Sulfolane				4.0	2c/125		
CS_2	29	40	1175	12.2	2a/35		
Acetic acid	None		1933	0.9	2a/48		
Aniline							
Nitrobenzene	None		2065				
Morpholine							
Pyridine	None		2024	1.0	2a/183		
2-Nitropropane	None		1977				
Acetonitrile	19	64	1925	2.4	2a/43		
Furfuraldehyde				1.0	2c/140		
Phenol							
Water	None		213	1.5	1/49		

Ethanol

Alternative names
Ethyl alcohol, grain alcohol, methylated spirits, IMS

Reference codes			
CAS number	64 17 5	Hazchem code	2SE
UN number	1170	EPA code	U001
Physical properties			
Molecular weight	46	Cubic expansion coeff (per °C × 10^3)	1.1
Empirical formula	$C_2H_6O_1$	Surface tension (@20°C dyn/cm)	22.3
Boiling point (°C)	78	Absolute viscosity (@25°C cP)	1.08
Freezing point (°C)	–114	Refractive index (25°C)	1.359
Specific gravity (20/4)	0.789		
Fire hazards			
Flash point (closed cup °C)	13	Lower explosive limit (ppm)	33000
Autoignition temperature (°C)	419	Upper explosive limit (ppm)	190000
Electrical conductivity	1.4E–9		
Health hazards			
IDLH (ppm)		Vapour concentration @21°C ppm	64000
OES-TWA	1000	Vapour density (relative to air)	1.6
OES-STEL		Vapour pressure @21°C mmHg	45.7
Odour Threshold (ppm)	6000	POCP	27
Aqueous effluent			
Solubility in water (25°C %w/w)		Total	
Solubility of water in (25°C %w/w)		Total	
Log_{10} activated carbon partition		1.35	
Log_{10} partition in octanol/water (w/w)		–0.32	
Biological oxygen demand w/w (days)		0.92 (5)	
Theoretical oxygen demand w/w		2.09	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	8.11220	
	B	1592.864	
	C	226.184	
Cox chart	A	8.24183	
	B	1651.2	
Solvent properties			
Solubility parameter	13.4	Kauri butanol value	325
Dipole (D)	1.7	Evaporation time (ether = 1)	8.3
Dielectric constant (20°C)	22.4	Evaporation time (BuAc = 1)	2.4
Polarity (water 100)	65.4		
Thermal information			
Latent heat (cal/mol)	9200		
Nett heat of combustion (kcal/gmol)	296		
Specific heat (cal/mol/°C)	27		
Critical pressure (MN/m^2)	6.39		
Critical temperature (K)	516		
Latent heat of fusion (cal/mol)	1198		
Van der Waals' volume	2.11		
Van der Waals' surface area	1.97		
Molar volume	58.68		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	5	34	4062	6.9	2c/375		
n-Hexane	21	59	4106	8.9	2a/353		
n-Heptane	72	98	4139	11.3	2a/498		
n-Octane	78	77	4165	15.1	2c/462		
n-Nonane				24.5	2e/398		
n-Decane				14.5	2a/508		
2,2,4-TMP	40	72	4167	10.8	2a/503		
Cyclohexane	31	65	4087	7.5	2a/430		
Benzene	32	68	4073	4.0	2a/399		
Toluene	63	77	4120	5.9	2a/477		
Ethylbenzene	None		4144	6.4	2c/460		
Xylenes	None		4146	7.7	2a/500		
C_9 Aromatics	None		4175				
Tetralin							
Alcohols							
Methanol	None		1944	1.1	2a/60		
Ethanol	–		–	–	–	–	–
n-Propanol	None		3981	1.1	2a/236		
i-Propanol	None		3980	1.0	2a/341		
n-Butanol	None		4026	1.0	2a/365		
i-Butanol	None		4029a				
s-Butanol	None		4027	1.0	2a/366		
n-Amyl alc.	None		4063	1.1	2a/396		
i-Amyl alc.	None		1066	1.3	2a/395		
Cyclohexanol	None			2.3	2c/421		
1-Octanol	None						
Ethanediol	None		6.5	2c/297			
DEG	None						
1,2-Propanediol	None		1.9	2c/319			
Glycol ethers							
PGME							
EGME	None		3982				
EEE	None		4032		2c/350		
EGBE	None						
Chlorinated							
MDC	2	40	1551	1.7	2c/283		
Chloroform	7	59	1442	2.0	2a/285		
Carbon tet.	16	65	1105	4.7	2a/276		
1,2-EDC	37	70	2964	3.6	2a/299		
1,1,1-TCA							
TCE	28	71	2286	4.7	2a/295		
Perk.	63	77	2162	6.1	2c/285		
MCB	None		4070	5.6	2a/397		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		3965	1.8	2a/321		
MEK	39	74	4005	1.7	2a/343		
MIBK	None		4101	2.1	2c/423		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	None		4029	2.6	2a/375		
DIPE	17	64	4110	4.1	2a/459		
Dibutyl ether	None		4170	5.0	2e/391		
MTBE							
1,4-Dioxane	>98	78	4011	2.2	2a/348		
THF	10		4009	1.5	2a/328		
Esters							
Me acetate	3	57	3969	1.9	2a/335		
Et acetate	26	72	4012	2.4	2a/351		
i-Propyl acetate	52	77	4054	2.1	2a/391		
n-Butyl acetate	None			3.1	2c/426		
Cellosolve acetate							
Miscellaneous							
DMF	None			0.7	2c/371		
DMAc							
DMSO							
Sulfolane				8.1	2c/344		
CS_2	9	43	1189	6.5	2a/281		
Acetic acid				0.7	2c/293		
Aniline	None		4075	4.9	2a/427		
Nitrobenzene	None		4072				
Morpholine				0.6	2c/345		
Pyridine	None		4038	1.0	2c/355		
2-Nitropropane	94	78	3978				
Acetonitrile	56	73	2760	1.9	2a/298		
Furfuraldehyde	None			5.5	2a/383		
Phenol							
Water	96	78	242	2.7	1/165		

n-Propanol

Alternative names
Propan-1-ol, *n*-propyl alcohol, 1-propanol, ethyl carbinol

Reference codes			
CAS number	71 23 8	Hazchem code	2SE
UN number	1274	EPA code	
Physical properties			
Molecular weight	60	Cubic expansion coeff (per °C × 10^3)	0.96
Empirical formula	$C_3H_8O_1$	Surface tension (@20°C dyn/cm)	23.7
Boiling point (°C)	97	Absolute viscosity (@25°C cP)	1.72
Freezing point (°C)	–127	Refractive index (25°C)	1.383
Specific gravity (20/4)	0.804		
Fire hazards			
Flash point (closed cup °C)	25	Lower explosive limit (ppm)	21000
Autoignition temperature (°C)	440	Upper explosive limit (ppm)	135000
Electrical conductivity	9.0E–9		
Health hazards			
IDLH (ppm)	4000	Vapour concentration @21°C ppm	18000
OES-TWA	200	Vapour density (relative to air)	2.07
OES-STEL	250	Vapour pressure @21°C mmHg	13.4
Odour threshold (ppm)	45	POCP	45
Aqueous effluent			
Solubility in water (25°C %w/w)		Total	
Solubility of water in (25°C %w/w)		Total	
Log_{10} activated carbon partition		1.67	
Log_{10} partition in octanol/water (w/w)		+0.34	
Biological oxygen demand w/w (days)		1.5	
Theoretical oxygen demand w/w		2.40	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	8.37895	
	B	1788.020	
	C	227.438	
Cox chart	A	8.25022	
	B	1755.8	
Solvent properties			
Solubility parameter	11.9	Kauri butanol value	250
Dipole (D)	1.7	Evaporation time (ether = 1)	9.0
Dielectric constant (20°C)	20.1	Evaporation time (BuAc = 1)	1.0
Polarity (water 100)	61.7		
Thermal information			
Latent heat (cal/mol)	9780		
Nett heat of combustion (kcal/gmol)	438		
Specific heat (cal/mol/°C)	34		
Critical pressure (MN/m^2)	5.10		
Critical temperature (K)	537		
Latent heat of fusion (cal/mol)	1240		
Van der Waals' volume	2.78		
Van der Waals' surface area	2.51		
Molar volume	75.14		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None		6484				
n-Hexane	4	66	6505	13.3	2a/584		
n-Heptane	36	88	6514	5.0	2a/596		
n-Octane	70	94	6523	6.6	2a/576		
n-Nonane	98	97		8.3	2e/505		
n-Decane	None			8.7	2a/606		
2,2,4-TMP	41	85	6524	6.5	2e/500		
Cyclohexane	20	74	6495	3.8	2a/579	1.2	CEH
Benzene	17	77	6491	3.3	2a.556		
Toluene	49	93	6512	3.3	2a/592		
Ethylbenzene	91	7	6517	3.8	2a/601		
Xylenes	93	97	6519	4.0	2c/575		
C_9 Aromatics	None		6529				
Tetralin							
Alcohols							
Methanol	None			1.1	2a/122		
Ethanol	None		3981	1.1	2a/336		
n-Propanol	–		–	–	–	–	–
i-Propanol	None			1.1	2a/531		
n-Butanol	None			1.1	2a/539	0.07	CEH
i-Butanol	None		6465	1.1	2a/541		
s-Butanol	None		6463				
n-Amyl alc.	None			1.0	2e/471		
i-Amyl alc.	None		6486	1.0	2a/548		
Cyclohexanol				1.8	2e/414		
1-Octanol							
Ethanediol	None		4195a	6.2	2c/483		
DEG							
1,2-Propanediol				2.9	2c/491		
Glycol ethers							
PGME							
EGME	None			1.3	2c/490		
EEE							
EGBE							
Chlorinated							
MDC	None			2.7	2e/416		
Chloroform	None		1454				
Carbon tet.	8	73	1116	3.3	2a/509		
1,2-EDC	19	81	2971	2.4	2a/520		
1,1,1-TCA	7	73					
TCE	17	82	2296	5.9	2a/518		
Perk.	48	94	2177				
MCB	80	97	6489	3.5	2a/552		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5320				
MEK	None		6445	1.6	2c/496		
MIBK	35	94					
Cyclohexanone							
NMP				0.2	2e/461		
Acetophenone							
Ethers							
Diethyl ether	None		6464				
DIPE	None			3.6	2a/586		
Dibutyl ether				3.2			
MTBE							
1,4-Dioxane	55	95	6447	1.8	2a/533		
THF	None			1.2	2c/497		
Esters							
Me acetate	None			3.6	2a/530		
Et acetate	None			1.7	2a/536		
i-Propyl acetate							
n-Butyl acetate	40	94		14.5	2e/484		
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc				0.4	2e/454		
DMSO							
Sulfolane							
CS_2	5	46	1209	3.6	2e/417		
Acetic acid				0.9	2a/525		
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	None		6469	0.8	2c/512		
2-Nitropropane	75	96	6271				
Acetonitrile	28	81	2768	3.0	2e/430		
Furfuraldehyde							
Phenol							
Water	71	87	293	3.95	1/301		

i-Propanol

Alternative names
Propan-2-ol, isopropyl alcohol, IPA – avoid confusion with IP acetate

Reference codes			
CAS number	67 63 0	Hazchem code	2SE
UN number	1219	EPA code	
Physical properties			
Molecular weight	60	Cubic expansion coeff (per °C × 10^3)	1.05
Empirical formula	$C_3H_8O_1$	Surface tension (@20°C dyn/cm)	21.7
Boiling point (°C)	82	Absolute viscosity (@25°C cP)	2.0
Freezing point (°C)	–88	Refractive index (25°C)	1.375
Specific gravity (20/4)	0.786		
Fire hazards			
Flash point (closed cup °C)	12	Lower explosive limit (ppm)	23000
Autoignition temperature (°C)	425	Upper explosive limit (ppm)	127000
Electrical conductivity	6.0E–8		
Health hazards			
IDLH (ppm)	20000	Vapour concentration @21°C ppm	46000
OES-TWA	400	Vapour density (relative to air)	2.07
OES-STEL	500	Vapour pressure @21°C mmHg	35.1
Odour threshold (ppm)	60	POCP	15
Aqueous effluent			
Solubility in water (25°C %w/w)		Total	
Solubility of water in (25°C %w/w)		Total	
Log_{10} activated carbon partition		1.46	
Log_{10} partition in octanol/water (w/w)		+0.26	
Biological oxygen demand w/w (days)		1.59	
Theoretical oxygen demand w/w		2.40	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	8.87829	
	B	2010.33	
	C	252.636	
Cox chart	A	8.24362	
	B	1673.2	
Solvent properties			
Solubility parameter	11.5	Kauri butanol value	230
Dipole (D)	1.66	Evaporation time (ether = 1)	11
Dielectric constant (20°C)	18.3	Evaporation time (BuAc = 1)	1.5
Polarity (water 100)	54.6		
Thermal information			
Latent heat (cal/mol)	9540		
Nett heat of combustion (kcal/gmol)	433		
Specific heat (cal/mol/°C)	37		
Critical pressure (MN/m^2)	4.76		
Critical temperature (K)	508		
Latent heat of fusion (cal/mol)	1282		
Van der Waals' volume	2.78		
Van der Waals' surface area	2.51		
Molar volume	76.92		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	6	35	6370				
n-Hexane	23	63	6390	5.0	2b/97		
n-Heptane	51	76	6399	7.4	2b/113		
n-Octane	84	82	6418	7.8	2b/115		
n-Nonane	Azeo			7.9	2f/95		
n-Decane	None			6.6	2b/118		
2,2,4-TMP	54	77	6419	4.8	2b/116		
Cyclohexane	32	69	6384	4.7	2b/84		
Benzene	33	72	6375	4.0	2b/65		
Toluene	69	81	6397	3.8	2b/108		
Ethylbenzene	None		6402	5.3	2d/95		
Xylenes	None		6404	5.0	2d/96		
C_9 Aromatics	None		6423	5.0	2d/97		
Tetralin							
Alcohols							
Methanol	None		1978a	0.9	2e/123		
Ethanol	None		3980	1.1	2a/341		
n-Propanol	None			1.02	2f/47		
i-Propanol	–		–	–		–	–
n-Butanol	None			1.6	2d/55		
i-Butanol	None			1.0	2d/56		
s-Butanol	None			1.1	2b/62		
n-Amyl alc.	None			0.82	2f/63		
i-Amyl alc.	None						
Cyclohexanol	None						
1-Octanol	None						
Ethanediol	None						
DEG	None						
1,2-Propanediol	None			2.6	2d/47		
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC	None		1561	2.31	2f/36		
Chloroform	4	61	1453	1.6	2d/40		
Carbon tet.	18	69	1115	3.3	2b/36		
1,2-EDC	43	75	2970				
1,1,1-TCA	None		2729				
TCE	30	75	2295	4.0	2d/43		
Perk.	70	82	2176	5.7	2d/42		
MCB	None		6373	4.9	2d/64		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5319	2.4	2b/43		
MEK	32	78	6335	1.5	2b/54		
MIBK	None		6386	1.7	2b/96		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	None		6351				
DIPE	15	66	6391	2.9	2b/101		
Dibutyl ether				3.9			
MTBE							
1,4-Dioxane	None		6337	1.7	2b/56		
THF	None		6335a	1.4	2b/55		
Esters							
Me acetate	None		5516	2.5	2b/50		
Et acetate	25	75	6338	1.7	2b/59		
i-Propyl acetate	52	80	6363	1.77	2f/59		
n-Butyl acetate	None			2.0	2d/75		
Cellosolve acetate							
Miscellaneous							
DMF	None						
DMAc							
DMSO				2.5	2f/39		
Sulfolane				13.6	2d/53		
CS_2	8	44	1208				
Acetic acid				0.6	2d/44		
Aniline							
Nitrobenzene							
Morpholine							
Pyridine				0.9	2d/57		
2-Nitropropane	96	82	6270				
Acetonitrile	48	75	2767	2.57	2f/40		
Furfuraldehyde							
Phenol							
Water	88	80	292	3.2	1/334		

n-Butanol

Alternative names
Butyl alcohol, 1-butanol, butanol, propyl carbinol

Reference codes			
CAS number	71 36 3	Hazchem code	3Y
UN number	1120	EPA code	U031
Physical properties			
Molecular weight	74	Cubic expansion coeff (per °C × 10^3)	0.79
Empirical formula	$C_4H_{10}O_1$	Surface tension (@20°C dyn/cm)	24.6
Boiling point (°C)	118	Absolute viscosity (@25°C cP)	3.0
Freezing point (°C)	–80	Refractive index (25°C)	1.397
Specific gravity (20/4)	0.810		
Fire hazards			
Flash point (closed cup °C)	35	Lower explosive limit (ppm)	14000
Autoignition temperature (°C)	360	Upper explosive limit (ppm)	112000
Electrical conductivity	9.1E–9		
Health hazards			
IDLH (ppm)	8000	Vapour concentration @21°C ppm	6300
OES-TWA	50	Vapour density (relative to air)	2.55
OES-STEL	50	Vapour pressure @21°C mmHg	4.8
Odour threshold (ppm)	5000	POCP	55

Aqueous effluent	
Solubility in water (25°C %w/w)	7.3
Solubility of water in (25°C %w/w)	20.4
Log_{10} activated carbon partition	2.36
Log_{10} partition in octanol/water (w/w)	+0.88
Biological oxygen demand w/w (days)	1.15 (5)
Theoretical oxygen demand w/w	2.21

Vapour pressure equation constants (Log_{10}, mmHg)		
Antoine equation	A	7.83800
	B	1558.19
	C	196.881
Cox chart	A	8.25925
	B	1871.7

Solvent properties			
Solubility parameter	11.4	Kauri butanol value	225
Dipole (D)	1.66	Evaporation time (ether = 1)	33
Dielectric constant (20°C)	18.2	Evaporation time (BuAc = 1)	0.47
Polarity (water 100)	60.2		

Thermal information	
Latent heat (cal/mol)	10434
Nett heat of combustion (kcal/gmol)	586
Specific heat (cal/mol/°C)	41
Critical pressure (MN/m^2)	4.41
Critical temperature (K)	563
Latent heat of fusion (cal/mol)	2215
Van der Waals' volume	3.45
Van der Waals' surface area	3.05
Molar volume	91.97

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None			4.1	2b/169		
n-Hexane	3	68	8163	2.8	2b/200		
n-Heptane	18	94	8182	4.2	2b/218		
n-Octane	50	110	8194	6.6	1x/3/1075		
n-Nonane	72	116	8203	10.0	2f/209		
n-Decane	8			8.9	2b/236		
2,2,4-TMP							
Cyclohexane	4	80	8146	3.3	2b/188		
Benzene	None		8136	2.1	2f/169		
Toluene	28	105	8170	2.3	2b/207		
Ethylbenzene	67	115	8185	2.7	2b/228		
Xylenes	73	115	8186	2.7	2b/229		
C_9 Aromatics	None		8198				
Tetralin				3.1	2b/235		
Alcohols							
Methanol	None		2015	1.3	2a/169	0.84	V2/99
Ethanol	None		4026	1.0	2a/365	0.34	V4/205
n-Propanol	None			1.0	2a/539	0.12	V4/226
i-Propanol	None			1.0	2d/55	0.24	V2/590
n-Butanol	–		–	–	–	–	–
i-Butanol	None		8103	1.0	2b/161	0.07	V3/110
s-Butanol	None		8102	0.9	2b/154		
n-Amyl alc.	None			1.0	2b/173		
i-Amyl alc.	None			1.1	2b/170		
Cyclohexanol	None			1.2	2b/193		
1-Octanol							
Ethanediol				2.6	2d/6	1.10	V2/420
DEG				1.8	2d/174		
1,2-Propanediol				1.8	2d/137		
Glycol ethers							
PGME							
EGME							
EEE	None		8106				
EGBE	None		8106	1.1	2f/189		
Chlorinated							
MDC				1.9	1x/1/130		
Chloroform	None			1.5	2b/136		
Carbon tet.	3	77	1133	2.4	2b/135		
1,2-EDC	None		2984	2.3	2b/137		
1,1,1-TCA				2.0	2f/123		
TCE	3	87	2306	2.8	2f/121		
Perk.	30	109	2186	3.1	2d/155		
MCB	56	115	8133	2.5	2b/175		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5344	1.1	2b/140	0.31	V2/469
MEK	None		7357	2.0	2b/143	0.14	V4/237
MIBK	30	114	8152	1.8	2d/193		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	None		8104	1.7	1x/3/1072		
DIPE	None			2.4	2b/202		
Dibutyl ether	83	118	8195	2.4	2d/231		
MTBE							
1,4-Dioxane	None			1.1	2b/147		
THF	None			1.2	2b/146		
Esters							
Me acetate				1.0	2f/137		
Et acetate	None			1.8	2b/148		
i-Propyl acetate	None		8121				
n-Butyl acetate	63	116	8153	1.7	2b/197		
Cellosolve acetate	None		8160				
Miscellaneous							
DMF							
DMAc							
DMSO	None			0.5	2f/131		
Sulfolane							
CS_2	None		1233	2.6	2f/120		
Acetic acid	57	120	3135	1.0	2d/158	0.20	P307
Aniline	None		8138				
Nitrobenzene	None		8135				
Morpholine							
Pyridine	70	119	8109	0.7	2b/166		
2-Nitropropane	48	112	6275				
Acetonitrile	None			4.1	2d/156		
Furfuraldehyde				3.2	2f/155		
Phenol							
Water	58	93	372	5.1	1/407		

i-Butanol

Alternative names
Isopropyl carbinol, isobutyl alcohol, IBA, 2-me-1-propanol

Reference codes			
CAS number	73 83 1	Hazchem code	3Y
UN number	1120	EPA code	U140
Physical properties			
Molecular weight	74	Cubic expansion coeff (per °C × 10^3)	0.95
Empirical formula	$C_4H_{10}O_1$	Surface tension (@20°C dyn/cm)	22.8
Boiling point (°C)	108	Absolute Viscosity (@25°C cP)	3.96
Freezing point (°C)	–108	Refractive index (25°C)	1.394
Specific gravity (20/4)	0.802		
Fire hazards			
Flash point (closed cup °C)	25	Lower explosive limit (ppm)	16000
Autoignition temperature (°C)	390	Upper explosive limit (ppm)	109000
Electrical conductivity	1.6E–8		
Health hazards			
IDLH (ppm)	8000	Vapour concentration @21°C ppm	11500
OES-TWA	50	Vapour density (relative to air)	2.56
OES-STEL	75	Vapour pressure @21°C mmHg	8.6
Odour threshold (ppm)	80	POCP	40
Aqueous effluent			
Solubility in water (25°C %w/w)		8.7	
Solubility of water in (25°C %w/w)		15.0	
Log_{10} activated carbon partition		2.16	
Log_{10} partition in octanol/water (w/w)		+0.74	
Biological oxygen demand w/w (days)		1.62	
Theoretical oxygen demand w/w		2.6	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	8.53516	
	B	1950.94	
	C	237.147	
Cox chart	A	8.25506	
	B	1816.5	
Solvent properties			
Solubility parameter	10.7	Kauri butanol value	
Dipole (D)	1.7	Evaporation time (ether = 1)	25
Dielectric constant (20°C)	17.7	Evaporation time (BuAc = 1)	0.6
Polarity (water 100)	55.2		
Thermal information			
Latent heat (cal/mol)	10220		
Nett heat of combustion (kcal/gmol)	585		
Specific heat (cal/mol/°C)	53		
Critical pressure (MN/m^2)	4.30		
Critical temperature (K)	548		
Latent heat of fusion (cal/mol)			
Van der Waals' volume	3.45		
Van der Waals' surface area	3.05		
Molar volume	92.91		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None		8327				
n-Hexane	2	68	8354	5.3	2f/320		
n-Heptane	27	91	8368	4.0	2f/326		
n-Octane		104	8377				
n-Nonane							
n-Decane							
2,2,4-TMP	27	92	8378				
Cyclohexane	14	78	8338	3.2	2f/317		
Benzene	8	79	8333	3.4	2f/316		
Toluene	45	101	8361	2.7	2b/289		
Ethylbenzene	80	107	8371				
Xylenes	88	107	8373	2.8	2b/292		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	None						
Ethanol	None		4029a				
n-Propanol	None		6465	0.9	2f/50	0.24	V2/552
i-Propanol	None			1.0	2d/56		
n-Butanol	None		8103	1.0	2f/153		
i-Butanol	–		–	–	–	–	–
s-Butanol	None			1.0	2f/223		
n-Amyl alc.	None			0.9	2f/311		
i-Amyl alc.	None		8328				
Cyclohexanol							
1-Octanol							
Ethanediol	None		2.3	2f/12			
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	None		6548				
EEE	None		8306				
EGBE							
Chlorinated							
MDC							
Chloroform	None		1475				
Carbon tet.	5	76	1137				
1,2-EDC	6	83	2988	2.1	2b/272		
1,1,1-TCA							
TCE	9	85	2309				
Perk.	40	103	2189				
MCB	63	107	8331	2.5	2d/357		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5347	1.4	2f/304		
MEK	None		7360				
MIBK	91	108	8343				
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether	None		8379				
MTBE							
1,4-Dioxane	4	101	7522	1.5	2b/278		
THF							
Esters							
Me acetate							
Et acetate	None		7570			0.03	P864
i-Propyl acetate	None		8318				
n-Butyl acetate	None		8345				
Cellosolve acetate	None		8352				
Miscellaneous							
DMF							
DMAc							
DMSO	None			0.4	2b/275		
Sulfolane							
CS_2	None		1236				
Acetic acid	Azeo			1.0	2f/302	0.21	P308
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	None		8307	0.7	2f/307	0.03	P1107
2-Nitropropane	67	105	6278				
Acetonitrile	None		2779	3.4	2f/300		
Furfuraldehyde							
Phenol							
Water	67	89	376	4.8	1/440		

s-Butanol

Alternative names
2-Butanol, methyl ethyl carbinol, 2-hydroxy-butane

Reference codes			
CAS number	78 92 2	Hazchem code	3Y
UN number	1120	EPA code	
Physical properties			
Molecular weight	74	Cubic expansion coeff (per °C × 10^3)	0.91
Empirical formula	$C_4H_{10}O_1$	Surface tension (@20°C dyn/cm)	23.0
Boiling point (°C)	99.5	Absolute viscosity (@25°C cP)	3.7
Freezing point (°C)	–115	Refractive index (25°C)	1.395
Specific gravity (20/4)	0.807		
Fire hazards			
Flash point (closed cup °C)	21	Lower explosive limit (ppm)	17000
Autoignition temperature (°C)	405	Upper explosive limit (ppm)	98000
Electrical conductivity	<1.0E–7		
Health hazards			
IDLH (ppm)	10,000	Vapour concentration @21°C ppm	17600
OES-TWA	100	Vapour density (relative to air)	2.56
OES-STEL	150	Vapour pressure @21°C mmHg	13.2
Odour threshold (ppm)	75	POCP	55
Aqueous effluent			
Solubility in water (25°C %w/w)		19.8	
Solubility of water in (25°C %w/w)		65.1	
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)		+0.61	
Biological oxygen demand w/w (days)		1.87	
Theoretical oxygen demand w/w		2.59	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.47429	
	B	1314.188	
	C	186.500	
Cox chart	A	8.25102	
	B	1766.8	
Solvent properties			
Solubility parameter	10.8	Kauri butanol value	195
Dipole (D)	1.7	Evaporation time (ether = 1)	13.0
Dielectric constant (20°C)	16.56	Evaporation time (BuAc = 1)	0.9
Polarity (water 100)	50.6		
Thermal information			
Latent heat (cal/mol)	9916		
Nett heat of combustion (kcal/gmol)	583		
Specific heat (cal/mol/°C)	40		
Critical pressure (MN/m^2)	4.20		
Critical temperature (K)	536		
Latent heat of fusion (cal/mol)			
Van der Waals' volume			
Van der Waals' surface area			
Molar volume	91.70		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None		8228				
n-Hexane	8	67	8242	4.3	2b/250		
n-Heptane	37	88	8248	3.8	2f/239		
n-Octane							
n-Nonane							
n-Decane				2.6	2b/285		
2,2,4-TMP	34	88	8254	4.1	2b/284		
Cyclohexane	18	76	8234	1.6	2f/234		
Benzene	15	79	8232	1.8	2f/227		
Toluene	55	95	8246	2.1	2b/276		
Ethylbenzene	None		8251				
Xylenes	None		8252	2.7	2b/282		
C_9 Aromatics				3.4	2f/241		
Tetralin							
Alcohols							
Methanol	None			0.9	2c/128		
Ethanol	None		4027	1.2	2a/366		
n-Propanol	None		6463				
i-Propanol	None			1.1	2b/62		
n-Butanol	None		8102	0.9	2b/154		
i-Butanol	None			1.0	2f/223		
s-Butanol	–		–	–	–	–	–
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	None		6547				
EEE							
EGBE							
Chlorinated							
MDC							
Chloroform	None		1472				
Carbon tet.	8	74	1134	2.2	2f/217		
1,2-EDC	12	82	2985	2.2	2f/220		
1,1,1-TCA							
TCE	15	84	2307	2.1	2f/219		
Perk.	57	97	2187	4.0	2b/240		
MCB	None		8230	2.7	2b/258		

Solute	Azeotrope X% w/w	°C)	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone							
MEK	None		7358	1.4	2b/239		
MIBK							
Cyclohexanone							
NMP							
Acetophenone				6.0	2b/251		
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane	40	99	7520				
THF							
Esters							
Me acetate							
Et acetate	None		7568				
i-Propyl acetate							
n-Butyl acetate	None		8237				
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2				4.8	2f/218		
Acetic acid				0.9	2f/221	0.20	P309
Aniline				3.8	2b/265		
Nitrobenzene	None		8231	12.5	2f/226		
Morpholine							
Pyridine	None		8217	0.8	2f/224		
2-Nitropropane	82	99	6276				
Acetonitrile				2.3	2b/241		
Furfuraldehyde							
Phenol							
Water	73	87	373	7.3	1/420		

n-Amyl alcohol

Alternative names
1-Pentanol, pentyl alcohol, butyl carbinol

Reference codes			
CAS number	71 41 0	Hazchem code	
UN number	1105	EPA code	
Physical properties			
Molecular weight	88	Cubic expansion coeff (per °C × 10^3)	0.92
Empirical formula	$C_5H_{12}O_1$	Surface tension (@20°C dyn/cm)	25.6
Boiling point (°C)	138	Absolute viscosity (@25°C cP)	4.0
Freezing point (°C)	–78	Refractive index (25°C)	1.408
Specific gravity (20/4)	0.815		
Fire hazards			
Flash point (closed cup °C)	48	Lower explosive limit (ppm)	11000
Autoignition temperature (°C)	360	Upper explosive limit (ppm)	100000
Electrical conductivity			
Health hazards			
IDLH (ppm)		Vapour concentration @21°C ppm	4030
OES-TWA		Vapour density (relative to air)	3.1
OES-STEL	150	Vapour pressure @21°C mmHg	3.0
Odour threshold (ppm)	10	POCP	
Aqueous effluent			
Solubility in water (25°C %w/w)		1.7	
Solubility of water in (25°C %w/w)		9.2	
Log_{10} activated carbon partition		2.74	
Log_{10} partition in octanol/water (w/w)		+1.40	
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w		2.73	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.3982	
	B	1435.57	
	C	179.8	
Cox chart	A		
	B		
Solvent properties			
Solubility parameter		Kauri butanol value	
Dipole (D)	1.7	Evaporation time (ether = 1)	
Dielectric constant (20°C)	13.9	Evaporation time (BuAc = 1)	0.3
Polarity (water 100)	56.8		
Thermal information			
Latent heat (cal/mol)	10613		
Nett heat of combustion (kcal/gmol)	733		
Specific heat (cal/mol/°C)	37		
Critical pressure (MN/m^2)	3.84		
Critical temperature (K)	586		
Latent heat of fusion (cal/mol)	2345		
Van der Waals' volume	4.13		
Van der Waals' surface area	3.59		
Molar volume	108.6		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ∞	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				3.8	1x/3/1154		
n-Hexane	None		9758	3.7	1x/3/1155		
n-Heptane	Azeo			4.8	2f/382		
n-Octane		122	9769	3.7	2f/383		
n-Nonane				4.5	1x/3/1156		
n-Decane							
2,2,4-TMP							
Cyclohexane	None		9752	3.3	1x/3/1155		
Benzene	None		9748	2.6	1x/3/1155		
Toluene	None		9760	3.1	1x/3/1156		
Ethylbenzene	40	130	9765				
Xylenes	42	131	9766				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	None		2056	1.3	2a/202	0.14	V2/117
Ethanol	None		4063	1.5	2a/396	0.50	V2/348
n-Propanol	None			1.0	2c/471		
i-Propanol	None			0.9	2f/63		
n-Butanol	None			0.8	2b/173		
i-Butanol				1.0	2f/311		
s-Butanol							
n-Amyl alc.	–		–	–	–	–	–
i-Amyl alc.	None		9746a				
Cyclohexanol							
1-Octanol							
Ethanediol	None			4.4	2d/8	2.7	V2/423
DEG							
1,2-Propanediol				1.7	2d/139		
Glycol ethers							
PGME							
EGME	None		6560				
EEE	None		8419				
EGBE							
Chlorinated							
MDC				1.8	1x/3/1153		
Chloroform				1.3	1x/3/1153		
Carbon tet.	None		1147a	1.7	2f/375		
1,2-EDC				1.2	2f/373		
1,1,1-TCA							
TCE							
Perk.	15	117	2201				
MCB	25	126	9747				

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				2.1	1x/3/1154		
MEK				1.8	1x/3/1154		
MIBK	Azeo			1.7	2f/380		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether				1.7	1x/3/1154		
DIPE							
Dibutyl ether	50	135	9770				
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate				2.1	1x/3/1154		
i-Propyl acetate							
n-Butyl acetate	None		9754				
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2	None		1257	2.0	2f/371	0.22	P313
Acetic acid							
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	None		8836				
2-Nitropropane	15	120	6280				
Acetonitrile							
Furfuraldehyde						0.05	V3/186
Phenol	None		9749			<0.01	P1649
Water	46	96	464	3.4	1a/383		

i-Amyl alcohol

Alternative names
Fusel oil, 3-methyl-1-butanol, isopentyl alcohol, isobutyl carbinol

Reference codes			
CAS number	123 51 3	Hazchem code	
UN number		EPA code	
Physical properties			
Molecular weight	88	Cubic expansion coeff (per °C × 10^3)	1.12
Empirical formula	$C_5H_{12}O_1$	Surface tension (@20°C dyn/cm)	23.8
Boiling point (°C)	130	Absolute viscosity (@25°C cP)	4.2
Freezing point (°C)	−134	Refractive index (25°C)	1.4014
Specific gravity (20/4)	0.810		
Fire hazards			
Flash point (closed cup °C)	46	Lower explosive limit (ppm)	12000
Autoignition temperature (°C)	365	Upper explosive limit (ppm)	90000
Electrical conductivity			
Health hazards			
IDLH (ppm)	8000	Vapour concentration @21°C ppm	3140
OES-TWA	100	Vapour density (relative to air)	3.06
OES-STEL	125	Vapour pressure @21°C mmHg	2.4
Odour threshold (ppm)	15	POCP	
Aqueous effluent			
Solubility in water (25°C %w/w)		2.75	
Solubility of water in (25°C %w/w)			
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)		+1.16	
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w		2.73	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.382	
	B	1373.8	
	C	174.3	
Cox chart	A		
	B		
Solvent properties			
Solubility parameter		Kauri butanol value	
Dipole (D)	1.8	Evaporation time (ether = 1)	62
Dielectric constant (20°C)	15.2	Evaporation time (BuAc = 1)	
Polarity (water 100)	56.5		
Thermal information			
Latent heat (cal/mol)	10542		
Nett heat of combustion (kcal/gmol)	792		
Specific heat (cal/mol/°C)	47.3		
Critical pressure (MN/m^2)			
Critical temperature (K)	583		
Latent heat of fusion (cal/mol)			
Van der Waals' volume	4.13		
Van der Waals' surface area	3.59		
Molar volume	109.2		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ°	Solute γ° Reference	Partition coefficient	Partition coefficient Reference
Hydrocarbons							
n-Pentane							
n-Hexane	None		9845				
n-Heptane	7	98	9869				
n-Octane	35	120	9881	4.8	1x/3/1151		
n-Nonane							
n-Decane							
2,2,4-TMP	5	99	9882				
Cyclohexane	None		9834				
Benzene	None		9821				
Toluene	10	110	9852	3.0	1x/3/1151		
Ethylbenzene	49	126	9871				
Xylenes	52	126	9873				
C_9 Aromatics	None		9887				
Tetralin							
Alcohols							
Methanol	None			1.2	2a/201		
Ethanol	None		4066	1.2	2a/395	0.50	V2/347
n-Propanol	None		6486	1.0	2a/548	0.12	V2/566
i-Propanol						0.07	V2/592
n-Butanol	None			1.0	2b/170		
i-Butanol	None		8328			0.08	V3/139
s-Butanol							
n-Amyl alc.							
i-Amyl alc.	–		–	–	–	–	–
Cyclohexanol							
1-Octanol							
Ethanediol	None		4221	4.1	2d/7		
DEG							
1,2-Propanediol	None			1.7	2d/138		
Glycol ethers							
PGME	None		9816				
EGME	None		6562				
EEE	None		8420				
EGBE							
Chlorinated							
MDC							
Chloroform							
Carbon tet.	None		1149				
1,2-EDC	None		2995				
1,1,1-TCA							
TCE	None		2321				
Perk.	19	116	2203				
MCB	34	124	9819				

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone							
MEK				1.8	1x/3/1151		
MIBK	None		9836				
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether	65	130	9883				
MTBE							
1,4-Dioxane				2.1	1x/3/1151		
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate	None		9842				
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	84	133	3156a				
Aniline	None		9824				
Nitrobenzene							
Morpholine							
Pyridine	None		8838				
2-Nitropropane							
Acetonitrile							
Furfuraldehyde						0.07	V3/185
Phenol	None		9822				
Water	50	95	468	1.9	1a/382		

Cyclohexanol

Alternative names
Hexalin, cyclohexyl alcohol

Reference codes

CAS number	108 93 0	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	100	Cubic expansion coeff (per °C × 10^3)	0.82
Empirical formula	$C_6H_{12}O_1$	Surface tension (@20°C dyn/cm)	32
Boiling point (°C)	161	Absolute viscosity (@25°C cP)	52.7
Freezing point (°C)	+25	Refractive index (25°C)	1.465
Specific gravity (20/4)	0.949		

Fire hazards

Flash point (closed cup °C)	68	Lower explosive limit (ppm)	20000
Autoignition temperature (°C)	300	Upper explosive limit (ppm)	
Electrical conductivity			

Health hazards

IDLH (ppm)	3500	Vapour concentration @21°C ppm	1500
OES-TWA	50	Vapour density (relative to air)	3.45
OES-STEL		Vapour pressure @21°C mmHg	1.14
Odour threshold (ppm)	1	POCP	

Aqueous effluent

Solubility in water (25°C %w/w)	4.3
Solubility of water in (25°C %w/w)	11.8
Log_{10} activated carbon partition	
Log_{10} partition in octanol/water (w/w)	+1.23
Biological oxygen demand w/w (days)	0.08 (5)
Theoretical oxygen demand w/w	2.83

Vapour pressure equation constants (Log_{10}, mmHg)

Antoine equation	A	8.35237
	B	2258.560
	C	251.624
Cox chart	A	8.27876
	B	2110.6

Solvent properties

Solubility parameter	11.4	Kauri butanol value	
Dipole (D)	1.8	Evaporation time (ether = 1)	150
Dielectric constant (20°C)	15.0	Evaporation time (BuAc = 1)	0.08
Polarity (water 100)	50.0		

Thermal information

Latent heat (cal/mol)	10900
Nett heat of combustion (kcal/gmol)	892
Specific heat (cal/mol/°C)	50
Critical pressure (MN/m^2)	3.7
Critical temperature (K)	625
Latent heat of fusion (cal/mol)	419
Van der Waals' volume	4.35
Van der Waals' surface area	3.51
Molar volume	103.43

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				5.5	1x/3/1232		
n-Hexane	None			5.7	1x/1/272		
n-Heptane	None		11727	6.8	2f/419		
n-Octane							
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	None		11684	3.4	1x/1/272		
Benzene	None		10856	2.7	1x/1/272		
Toluene	None		11720				
Ethylbenzene							
Xylenes	10	140	11730		2f/536		
C_9 Aromatics	40		11750				
Tetralin							
Alcohols							
Methanol							
Ethanol	None			1.2	2c/421		
n-Propanol	None			3.9	2e/414		
i-Propanol	None						
n-Butanol	None			1.0	2b/193		
i-Butanol							
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol	–		–	–	–	–	–
1-Octanol							
Ethanediol	None		4257	2.3	2d/14		
DEG							
1,2-Propanediol							
Glycol ethers							
PGME	None		9967				
EGME							
EEE							
EGBE	None		11712			0.02	P3974
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB	None			1.6	2b/393		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Part coefficient	Reference
Ketones							
Acetone	None			3.8	2d/510		
MEK							
MIBK							
Cyclohexanone	None		11357		2b/395		
NMP				0.5	2f/411		
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether	None		11745				
MTBE							
1,4-Dioxane	None		7543				
THF							
Esters							
Me acetate							
Et acetate	None			1.4	2d/511		
i-Propyl acetate							
n-Butyl acetate	None			1.3	2f/417		
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid						0.24	V/260
Aniline	None		11149	1.4	2f/416		
Nitrobenzene							
Morpholine							
Pyridine						0.05	V3/234
2-Nitropropane							
Acetonitrile							
Furfuraldehyde	95	156	8764				
Phenol	13	183	10895	2.8	2b/385		
Water	30	98	528	4.5	1/514		

n-Octanol

Alternative names
Octyl alcohol, heptyl carbinol

Reference codes

CAS number	111 87 5	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	130	Cubic expansion coeff (per °C × 10^3)	0.99
Empirical formula	$C_8H_{18}O_1$	Surface tension (@20°C dyn/cm)	27.5
Boiling point (°C)	194	Absolute viscosity (@25°C cP)	7.5
Freezing point (°C)	–16	Refractive index (25°C)	1.427
Specific gravity (20/4)	0.827		

Fire hazards

Flash point (closed cup °C)	81	Lower explosive limit (ppm)	30000
Autoignition temperature (°C)		Upper explosive limit (ppm)	
Electrical conductivity	1.4E–7		

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	186
OES-TWA		Vapour density (relative to air)	4.5
OES-STEL		Vapour pressure @21°C mmHg	0.14
Odour threshold (ppm)	0.5	POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		0.6
Solubility of water in (25°C %w/w)		
Log_{10} activated carbon partition		
Log_{10} partition in octanol/water (w/w)		3.15
Biological oxygen demand w/w (days)		2.95 (5)
Theoretical oxygen demand w/w		2.95

Vapour pressure equation constants (Log_{10}, mmHg)

Antoine equation	A	6.5422
	B	1139.45
	C	115.9
Cox chart	A	8.29377
	B	2295.1

Solvent properties

Solubility parameter	10.4	Kauri butanol value	
Dipole (D)	1.9	Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)	54.3		

Thermal information

Latent heat (cal/mol)	12675
Nett heat of combustion (kcal/gmol)	1167
Specific heat (cal/mol/°C)	65
Critical pressure (MN/m^2)	2.69
Critical temperature (K)	659
Latent heat of fusion (cal/mol)	
Van der Waals' volume	6.15
Van der Waals' surface area	5.21
Molar volume	158.4

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				2.6	1x/1/401		
n-Hexane				2.8	1x/1/402		
n-Heptane				3.1	1x/1/402		
n-Octane				3.4	1x/1/402		
n-Nonane							
n-Decane				2.8	2f/542		
2,2,4-TMP							
Cyclohexane							
Benzene				2.1	1x/1/401	<0.01	P1483
Toluene				2.1	1x/1/402	<0.01	P2286
Ethylbenzene				2.5	1x/1/402	<0.01	P2874
Xylenes	None		14113	2.4	1x/1/402	<0.01	P2876
C_9 Aromatics	None		14728	2.7	1x/1/402		
Tetralin	87	194		1.4	2f541		
Alcohols							
Methanol						0.76	P155
Ethanol				1.1	1x/3/1371	0.29	P367
n-Propanol						0.06	P636
i-Propanol							
n-Butanol						0.02	P947
i-Butanol						0.03	P964
s-Butanol						0.03	P973
n-Amyl alc.						<0.01	P1266
i-Amyl alc.						<0.01	P1273
Cyclohexanol						<0.01	P1894
1-Octanol	–		–	–	–	–	–
Ethanediol	63	184	4356				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE						0.48	P1000
EGBE						0.01	P3976
Chlorinated							
MDC				1.6	1x/1/401		
Chloroform				1.0	1x/1/401	<0.01	P87
Carbon tet.				1.7	1x/1/401		
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB						<0.01	P1377

Solute	Azeotrope X w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				2.6	1x/1/401	0.24	P491
MEK				2.0	1x/1/401	0.07	P852
MIBK							
Cyclohexanone						0.02	P1839
NMP							
Acetophenone	87	195	13909			<0.01	P2743
Ethers							
Diethyl ether						0.04	P986
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				1.2	1x/3/1371		
THF							
Esters							
Me acetate						0.09	P515
Et acetate				2.4	1x/1/401		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF				1.23	2f/527		
DMAc						0.82	P931
DMSO						14.8	P386
Sulfolane							
CS_2				1.8	1x/1/401		
Acetic acid						0.24	P282
Aniline	17	184	11200			0.02	P1710
Nitrobenzene	None		10754			<0.01	P1438
Morpholine						1.66	P932
Pyridine						0.07	V3/234
2-Nitropropane							
Acetonitrile				7.5	1x/1/401	0.30	P260
Furfuraldehyde	None		8789				
Phenol	87	195	10962			<0.01	P1617
Water	10	99	741				

Ethanediol

Alternative names
Glycol, monoethyleneglycol, 1,2-dihydroxyethane, MEG, **not** ethyl glycol

Reference codes

CAS number	107 21 1	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	62	Cubic expansion coeff (per °C × 10^3)	0.64
Empirical formula	$C_2H_6O_2$	Surface tension (@20°C dyn/cm)	46.5
Boiling point (°C)	198	Absolute viscosity (@25°C cP)	20
Freezing point (°C)	–13	Refractive index (25°C)	1.429
Specific gravity (20/4)	1.115		

Fire hazards

Flash point (closed cup °C)	111	Lower explosive limit (ppm)	32000
Autoignition temperature (°C)	413	Upper explosive limit (ppm	
Electrical conductivity	1.2E–6		

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	153
OES-TWA	60	Vapour density (relative to air)	2.15
OES-STEL	125	Vapour pressure @21°C mmHg	0.12
Odour threshold (ppm)		POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		Total
Solubility of water in (25°C %w/w)		Total
Log_{10} activated carbon partition		1.16
Log_{10} partition in octanol/water (w/w)		–1.93
Biological oxygen demand w/w (days)		0.16 (5)
Theoretical oxygen demand w/w		1.29

Vapour pressure equation constants (Log_{10}, mmHg)

Antoine equation	A	8.09083
	B	2088.936
	C	203.454
Cox chart	A	
	B	

Solvent properties

Solubility parameter	14.6	Kauri butanol value	
Dipole (D)	2.31	Evaporation time (ether = 1)	1550
Dielectric constant (20°C)	37.7	Evaporation time (BuAc = 1)	
Polarity (water 100)	79.0		

Thermal information

Latent heat (cal/mol)	12524
Nett heat of combustion (kcal/gmol)	250
Specific heat (cal/mol/°C)	35
Critical pressure (MN/m^2)	7.7
Critical temperature (K)	647
Latent heat of fusion (cal/mol)	2682
Van der Waals' volume	2.41
Van der Waals' surface area	2.25
Molar volume	55.92

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				229.0	1x/1/33		
n-Hexane	None		4265	384.0	1x/1/35		
n-Heptane	3	98	4312	806.0	1x/1/35		
n-Octane	11	124	4353	1170.0	1x/1/36		
n-Nonane				1710.0	1x/1/37		
n-Decane	23	161	4434	1970.0	1x/1/37		
2,2,4-TMP							
Cyclohexane	None		4255	148.0	1x/1/34		
Benzene	None		4239	45.7	1x/1/34		
Toluene	6	110	4285	76.9	1x/1/35		
Ethylbenzene	13	133	4321	86.7	1x/1/36		
Xylenes	16	140	4323	110.0	1x/1/36		
C_9 Aromatics		160	4372	200	1x/1/37		
Tetralin							
Alcohols							
Methanol	None		1946		2a/62		
Ethanol	None			2.1	2c/297		
n-Propanol	None		4195a	4.4	2c/483		
i-Propanol							
n-Butanol	None		4213	6.6	2d/6		
i-Butanol				2.5	2f/12		
s-Butanol							
n-Amyl alc.	None			4.1	2d/8		
i-Amyl alc.	None		4221	3.3	2d/7		
Cyclohexanol	None		4257	2.3	2d/14		
1-Octanol	36	184	4356				
Ethanediol	–		–	–	–	–	–
DEG				1.9	2f/13		
1,2-Propanediol				0.9	2b/12		
Glycol ethers							
PGME	None		4222				
EGME							
EEE							
EGBE	None		4268				
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE	None		2287				
Perk.	6	119	2163				
MCB	6	130	4233				

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				6.2	1x/3/971		
MEK				8.4	1x/3/971		
MIBK							
Cyclohexanone							
NMP				0.44	2f/17		
Acetophenone	52	186	4316				
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether	10	140	4354				
MTBE							
1,4-Dioxane	None		4206				
THF	None		4204a	3.60	2d/3		
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate	None		4258				
Cellosolve acetate	None		4261	6.9	2d/15		
Miscellaneous							
DMF				1.5	2b/8		
DMAc							
DMSO				0.5	2b/7		
Sulfolane							
CS_2							
Acetic acid							
Aniline	24	181	4242	3.9	2b/16		
Nitrobenzene	59	186	4238				
Morpholine							
Pyridine	None		4215				
2-Nitropropane							
Acetonitrile				5.1	2f/1		
Furfuraldehyde	None		4214				
Phenol	78	199	4240	1.1	2d/11		
Water	None		244	0.72	1a/173		

Diethylene glycol

Alternative names
DEG, 2,2-oxydiethanol

Reference codes

CAS number	111 46 6	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	106	Cubic expansion coeff (per °C × 10^3)	0.63
Empirical formula	$C_4H_{10}O_3$	Surface tension (@20°C dyn/cm)	48.5
Boiling point (°C)	245	Absolute viscosity (@25°C cP)	34
Freezing point (°C)	–8	Refractive index (25°C)	1.445
Specific gravity (20/4)	1.118		

Fire hazards

Flash point (closed cup °C)	124	Lower explosive limit (ppm)	16000
Autoignition temperature (°C)	229	Upper explosive limit (ppm)	108000
Electrical conductivity	6E–7		

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	25
OES-TWA		Vapour density (relative to air)	3.68
OES-STEL		Vapour pressure @21°C mmHg	0.019
Odour threshold (ppm)		POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		Total
Solubility of water in (25°C %w/w)		Total
Log_{10} activated carbon partition		1.86
Log_{10} partition in octanol/water (w/w)		–1.98
Biological oxygen demand w/w (days)		0.06 (5)
Theoretical oxygen demand w/w		1.51

Vapour pressure equation constants (Log_{10}, mmHg)

Antoine equation	A	12.83
	B	7046.4
	C	463.2
Cox chart	A	
	B	

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)	2.31	Evaporation time (ether = 1)	
Dielectric constant (20°C)	31.7	Evaporation time (BuAc = 1)	
Polarity (water 100)	71.3		

Thermal information

Latent heat (cal/mol)	15900
Nett heat of combustion (kcal/gmol)	567
Specific heat (cal/mol/°C)	58.4
Critical pressure (MN/m^2)	4.7
Critical temperature (K)	680
Latent heat of fusion (cal/mol)	
Van der Waals' volume	4.00
Van der Waals' surface area	3.57
Molar volume	94.8

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				64.1	1x/1/139		
n-Hexane				91.5	1x/1/141		
n-Heptane				95.6	1x/1/142		
n-Octane				139.8	1x/1/144		
n-Nonane				200.3	1x/1/144		
n-Decane				287.1	1x/1/145		
2,2,4-TMP				195.0	1x/1/144		
Cyclohexane				32.1	1x/1/140		
Benzene	None		8520	5.8	1x/1/139		
Toluene	None		8531	12.3	2f/341		
Ethylbenzene	Azeo		8545	14.9	1x/1/143		
Xylenes	Azeo		8547	17.0	1x/1/143		
C_9 Aromatics				25.0	1x/1/144		
Tetralin							
Alcohols							
Methanol				0.92	1x/3/1079		
Ethanol				1.3	1x/3/1079		
n-Propanol				1.5	1x/3/1079		
i-Propanol				1.4	1x/3/1080		
n-Butanol				1.9	1x/3/1080		
i-Butanol				1.7	1x/3/1080		
s-Butanol							
n-Amyl alc.				2.5	1x/3/1080		
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG	–		–	–	–	–	–
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB							

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				3.1	1x/3/1079		
MEK				3.7	1x/3/1080		
MIBK				8.0	1x/3/1081		
Cyclohexanone							
NMP							
Acetophenone	None		8538				
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				2.5	1x/3/1080		
THF							
Esters							
Me acetate				3.4	1x/3/1079		
Et acetate				5.3	1x/3/1080		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid							
Aniline							
Nitrobenzene	10	210	8518				
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde							
Phenol				0.6	2f/339		
Water	None		386	2.3	1a/353		

1,2-Propanediol

Alternative names
Propylene glycol, **not** propyl glycol

Reference codes

CAS number	57 55 6	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	76	Cubic expansion coeff (per °C × 10^3)	0.72
Empirical formula	$C_3H_8O_2$	Surface tension (@20°C dyn/cm)	72
Boiling point (°C)	187	Absolute viscosity (@25°C cP)	54
Freezing point (°C)	–60	Refractive index (25°C)	1.431
Specific gravity (20/4)	1.0362		

Fire hazards

Flash point (closed cup °C)	99	Lower explosive limit (ppm)	26000
Autoignition temperature (°C)	421	Upper explosive limit (ppm)	125000
Electrical conductivity	6.0E–7		

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	212
OES-TWA	150	Vapour density (relative to air)	2.52
OES-STEL		Vapour pressure @21°C mmHg	0.16
Odour threshold (ppm)		POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		Total
Solubility of water in (25°C %w/w)		Total
Log_{10} activated carbon partition		1.43
Log_{10} partition in octanol/water (w/w)		–1.35
Biological oxygen demand w/w (days)		
Theoretical oxygen demand w/w		1.68

Vapour pressure equation constants (Log_{10}, mmHg)

Antoine equation	A	8.9545
	B	2692.2
	C	255.2
Cox chart	A	
	B	

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)		Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	0.01
Polarity (water 100)	72.2		

Thermal information

Latent heat (cal/mol)	12844
Nett heat of combustion (kcal/gmol)	436
Specific heat (cal/mol/°C)	45
Critical pressure (MN/m^2)	6.1
Critical temperature (K)	624
Latent heat of fusion (cal/mol)	
Van der Waals' volume	3.28
Van der Waals' surface area	2.78
Molar volume	73.7

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane				120	1x/1/68		
n-Heptane				170	1x/1/68		
n-Octane				246	1x/1/68		
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane				58.9	1x/1/68		
Benzene	None		6654	16.2	1x/1/68		
Toluene	2	110	6658	26.4	1x/1/68		
Ethylbenzene							
Xylenes	10	136	6665				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol							
Ethanol				1.1	2c/319		
n-Propanol				1.4	2c/491		
i-Propanol				1.5	2d/47		
n-Butanol				1.7	2d/137		
i-Butanol							
s-Butanol							
n-Amyl alc.				2.2	2d/139		
i-Amyl alc.				1.7	2d/138		
Cyclohexanol							
1-Octanol							
Ethanediol				0.9	2b/12		
DEG							
1,2-Propanediol	–	–	–	–	–	–	
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB							

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone							
MEK							
MIBK							
Cyclohexanone							
NMP							
Acetophenone		183	6664				
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether		136	6668				
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate				3.1	2d/135		
i-Propyl acetate							
n-Butyl acetate	None		6655a				
Cellosolve acetate	None		6656				
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid							
Aniline	43	180	6655				
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde							
Phenol							
Water	None		296	1.2	1x/3/1013		