Section 1

Hydrocarbons

n-Pentane

Alternative names
Below 40°C, petroleum ether

Reference codes			
CAS number	109 66 0	Hazchem code	3Y
UN number	1265	EPA code	
Physical properties			
Molecular weight	72	Cubic expansion coeff (per °C × 10^3)	1.52
Empirical formula	C_5H_{12}	Surface tension (@20°C dyn/cm)	16
Boiling point (°C)	36	Absolute viscosity (@25°C cP)	0.235
Freezing point (°C)	–129	Refractive index (20°C)	1.358
Specific gravity (20/4)	0.626		
Fire hazards			
Flash point (closed cup °C)	–40	Lower explosive limit (ppm)	15000
Autoignition temperature (°C)	260	Upper explosive limit (ppm)	78000
Electrical conductivity	2E–10		
Health hazards			
IDLH (ppm)	5000	Vapour concentration @21°C ppm	768000
OES-TWA	600	Vapour density (relative to air)	2.5
OES-STEL	750	Vapour pressure @21°C mmHg	442
Odour threshold (ppm)	900	POCP	41
Aqueous effluent			
Solubility in water (25°C %w/w)		38E–4	
Solubility of water in (25°C %w/w)		120E–4	
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)		+3.23	
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w		3.56	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	6.87632	
	B	1075.780	
	C	233.205	
Cox chart	A	6.82847	
	B	1050.1	
Solvent properties			
Solubility parameter	7.0	Kauri butanol value	28
Dipole (D)	0	Evaporation time (ether = 1)	1.0
Dielectric constant (20°C)	1.844	Evaporation time (BuAc = 1)	13
Polarity (water 100)	0.9		
Thermal information			
Latent heat (cal/mol)	6120		
Nett heat of combustion (kcal/gmol)	776		
Specific heat (cal/mol/°C)	40.32		
Critical pressure (MN/m^2)	3.31		
Critical temperature (K)	470		
Latent heat of fusion (cal/mol)	2008		
Van der Waals' volume	3.825		
Van der Waals' surface area	3.316		
Molar volume	115.0		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	–		–	–	–	–	–
n-Hexane	None			0.9	6a/123		
n-Heptane	None			0.8	6a/127		
n-Octane				1.2	1x3/1149		
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	None		9742	1.1	6a/119		
Benzene	None		9741	1.6	6a118		
Toluene	None			3.5	6c/160		
Ethylbenzene							
Xylenes							
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	8	31	2055	19.0	2e/132		
Ethanol	95	34	4062	13.6	2c/375		
n-Propanol	None		6484				
i-Propanol	94	35	6370				
n-Butanol	None			8.5	2b/169		
i-Butanol	None		8327				
s-Butanol	None		8228				
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol	None			8.7	2f/529		
Ethanediol	None						
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC	51	3	1571	2.4	6a/100		
Chloroform	None		1482				
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	80	32	5368	7.1	3+4/190	0.91	V2/475
MEK				5.3	1x/3/1149		
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	32	33	8296				
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				4.8	1x/3/1149		
THF	None			2.2	1x/3/1149		
Esters							
Me acetate	78	34	5536				
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2	89	36	1256				
Acetic acid	None		3156				
Aniline							
Nitrobenzene	None		9740				
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile	90	35	2792	22.0	6a/102		
Furfuraldehyde							
Phenol							
Water	99	35	462				

n-Hexane

Alternative names
62/68 Hexane

Reference codes			
CAS number	110 54 3	Hazchem code	3YE
UN number	1208	EPA code	
Physical properties			
Molecular weight	86	Cubic expansion coeff (per °C × 10^3)	1.3
Empirical formula	C_6H_{14}	Surface tension (@20°C dyn/cm)	18.4
Boiling point (°C)	69	Absolute viscosity (@25°C cP)	0.31
Freezing point (°C)	–95	Refractive index (25°C)	1.372
Specific gravity (20/4)	0.659		
Fire hazards			
Flash point (closed cup °C)	–22	Lower explosive limit (ppm)	12000
Autoignition temperature (°C)	225	Upper explosive limit (ppm)	75000
Electrical conductivity	1.0E–16		
Health hazards			
IDLH (ppm)	5000	Vapour concentration @21°C ppm	170000
OES-TWA	20	Vapour density (relative to air)	2.99
OES-STEL		Vapour pressure @21°C mmHg	128
Odour threshold (ppm)		POCP	42
Aqueous effluent			
Solubility in water (25°C %w/w)		9.5E–4	
Solubility of water in (25°C %w/w)		110E–4	
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)		+3.80	
Biological oxygen demand w/w (days)		0.04 (7)	
Theoretical oxygen demand w/w		3.53	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	6.91058	
	B	1189.64	
	C	226.28	
Cox chart	A	6.9386	
	B	1212.1	
Solvent properties			
Solubility parameter	6.9	Kauri butanol value	30
Dipole (D)	0	Evaporation time (ether = 1)	1.4
Dielectric constant (20°C)	1.9	Evaporation time (BuAc = 1)	8.4
Polarity (water 100)	0.9		
Thermal information			
Latent heat (cal/mol)	6880		
Nett heat of combustion (kcal/gmol)	921		
Specific heat (cal/mol/°C)	42.0		
Critical pressure (MN/m^2)	3.03		
Critical temperature (K)	507.5		
Latent heat of fusion (cal/mol)	3119		
Van der Waals' volume	4.50		
Van der Waals' surface area	3.86		
Molar volume	130.5		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None			0.9	6a/123		
n-Hexane	–		–	–	–	–	
n-Heptane	None		12133	0.9	6a/604		
n-Octane	None		12134	0.5	6a/613		
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	None		11690	1.1	6a/273		
Benzene			10861	1.4	6a/535		
Toluene	None		12131	1.4	6a/591		
Ethylbenzene	None						
Xylenes	None			1.5	6a/605		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	72	50	2087	39.1	2a/253		
Ethanol	79	59	4106	12.3	2a/453	38.1	P383
n-Propanol	96	66	6506	22.4	2a/584	0.74	V2/577
i-Propanol	77	63	6390	10.5	2b/97	1.00	V2/616
n-Butanol	97	68	8163	11.2	2b/200	0.04	V3/121
i-Butanol	98	68	8354	13	2b/320		
s-Butanol	92	67	8242	9.5	2b/250		
n-Amyl alc.	None		9758				
i-Amyl alc.	None		9845				
Cyclohexanol	None						
1-Octanol				6.0	2f/532		
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	None						
EEE	95	66	8442	575.0	2b/295		
EGBE							
Chlorinated							
MDC	None		1575				
Chloroform	16	60	1495	1.3	6a/426		
Carbon tet.	None			1.2	6a/403		
1,2-EDC	None						
1,1,1-TCA	71	67	2730b	1.3	6a/473		
TCE	None		2330	1.5	6a/463		
Perk.	None		2217a	1.4	6a/453		
MCB	None		10519	1.8	6a/529		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	41	50	5385	4.2	3+4/225	0.8	V2/487
MEK	71	64	7376	3.5	3+4/302	0.13	V3/26
MIBK							
Cyclohexanone							
NMP							
Acetophenone				17.6	3b/451		
Ethers							
Diethyl ether	None						
DIPE	47	67	12128				
Dibutyl ether							
MTBE				1.2	1x/3/1240		
1,4-Dioxane	98	60		3.0	3+4/472		
THF	50	63		1.6	1x/3/1240	0.16	
Esters							
Me acetate	39	52					
Et acetate	62	65	7588	2.6	5/514		
i-Propyl acetate	91	69	9297				
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF	None				6c/332	24.8	V2/547
DMAc	None						
DMSO							
Sulfolane				121	1x/3/1240		
CS_2	None		1274				
Acetic acid	95	68	3184	13.4	5/152	9.2	V2/282
Aniline	None		11151	11.6	6a/580		
Nitrobenzene	None		10708	14.5	6a/532		
Morpholine							
Pyridine	None						
2-Nitropropane	97	69	6284	7.4	6a/510		
Acetonitrile	72	52	2800				
Furfuraldehyde							
Phenol						1.91	P1659
Water	94	62	570				

n-Heptane

Alternative names

Reference codes

CAS number	142 82 5	Hazchem code	3YE
UN number	1206	EPA code	

Physical properties

Molecular weight	100	Cubic expansion coeff (per °C × 10^3)	1.3
Empirical formula	C_7H_{16}	Surface tension (@20°C dyn/cm)	19.3
Boiling point (°C)	98	Absolute viscosity (@25°C cP)	0.41
Freezing point (°C)	–91	Refractive Index (25°C)	1.385
Specific gravity (20/4)	0.664		

Fire hazards

Flash point (closed cup °C)	–4	Lower explosive limit (ppm)	10000
Autoignition temperature (°C)	215	Upper explosive limit (ppm)	70000
Electrical conductivity	1.0E–16		

Health hazards

IDLH (ppm)	4250	Vapour concentration @21°C ppm	55000
OES-TWA	400	Vapour density (relative to air)	3.57
OES-STEL	500	Vapour pressure @21°C mmHg	40
Odour threshold (ppm)	150	POCP	53

Aqueous effluent

Solubility in water (25°C %w/w)	3E–4
Solubility of water in (25°C %w/w)	100E–4
Log_{10} activated carbon partition	
Log_{10} partition in octanol/water (w/w)	+3.5
Biological oxygen demand w/w (days)	0 (7)
Theoretical oxygen demand w/w	3.52

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

Antoine equation	A	6.89386
	B	1264.370
	C	216.64
Cox chart	A	7.04265
	B	1365.1

Solvent properties

Solubility parameter	7.5	Kauri butanol value	31
Dipole (D)	0.0	Evaporation time (ether = 1)	3.0
Dielectric constant (20°C)	1.924	Evaporation time (BuAc = 1)	3.3
Polarity (water 100)	1.2		

Thermal information

Latent heat (cal/mol)	7560
Nett heat of combustion (kcal/gmol)	1067
Specific heat (cal/mol/°C)	52
Critical pressure (MN/m^2)	2.74
Critical temperature (K)	540
Latent heat of fusion (cal/mol)	3378
Van der Waals' volume	5.17
Van der Waals' surface area	4.40
Molar volume	147.5

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.3	6a/127		
n-Hexane	None		12133	0.9	6a/604		
n-Heptane	–		–	–	–	–	–
n-Octane				1.0	6b/196		
n-Nonane							
n-Decane							
2,2,4-TMP	None		13809	1.0	6b/197		
Cyclohexane	None		11697	1.1	6a/304		
Benzene	0.7	80	10876	1.3	6b/123	<0.001	P1487
Toluene	None		13027	1.4	6b/169	0.003	P2290
Ethylbenzene	None		13807	1.7	6c/489	<0.001	P2877
Xylenes	None		13808	1.4	6c/497	<0.001	P2877
C_9 Aromatics				1.3	6b/200		
Tetralin							
Alcohols							
Methanol	59	49	2101	18.4	2c/243		
Ethanol	51	71	4139	11.6	2a/498	5.41	V2/376
n-Propanol	64	88	6514	15.5	2a/596	0.46	V2/583
i-Propanol	50	76	6399	14.5	2b/113	1.18	V2/620
n-Butanol	82	94	8182	7.6	2b/218		
i-Butanol	73	91	8368		2d/378		
s-Butanol	62	89	8248	8.0	2d/281		
n-Amyl alc.	Azeo			19.0	2f/382		
i-Amyl alc.	93	98	9869				
Cyclohexanol	None		11727	23.7	2f/419		
1-Octanol				8.2	2f/535		
Ethanediol	97	98	4312				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	77	92	6592	10.0	1x/1/359		
EEE	86	97	8461			0.90	P3982
EGBE							
Chlorinated							
MDC				2.2	1x/1/357		
Chloroform				1.3	6b/77		
Carbon tet.	None		1167	1.2	6b/67		
1,2-EDC	24	81	3009	2.3	6c/444		
1,1,1-TCA							
TCE	None		2335	1.3	1x/3/1328		
Perk.							
MCB	None		10531	1.7	6b/119		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	10	56	6393	3.1	3+4/242	0.66	CEH
MEK	30	77	7384	3.9	3+4/311	0.13	V3/29
MIBK	87	98	11801	2.5	3b/550		
Cyclohexanone				3.8	3b/509		
NMP				10.2	3b/460		
Acetophenone							
Ethers							
Diethyl ether				1.2	1x/3/1330		
DIPE	None		12196	4.2	3+4/559		
Dibutyl ether				1.0	3+4/592		
MTBE				1.2	1x/3/1331		
1,4-Dioxane	56	92	7552	2.7	3+4/478		
THF				1.4	1x/3/1330	0.08	V4/240
Esters							
Me acetate	3	57	5558	4.2	1x/1/358		
Et acetate	6	77	7594	3.5	1x/1/359		
i-Propyl acetate	33	88	9302				
n-Butyl acetate	None		11826a	2.0	5/591		
Cellosolve acetate							
Miscellaneous							
DMF	95	97		17.0	6b/98		
DMAc							
DMSO							
Sulfolane				108	1x/3/1330		
CS_2	None		1278	1.3	1x/1/357		
Acetic acid				18.1	5/175	10.4	V4/201
Aniline	None		11179	13.1	6b/161	0.20	P1722
Nitrobenzene							
Morpholine							
Pyridine	75	96	8860	3.1	6b/116		
2-Nitropropane	79	95	6289	5.0	6b/100		
Acetonitrile	54	69	2803	25.7	6b/79		
Furfuraldehyde	95	98	8781	10.6	3+4/50		
Phenol	None		10936	20.0	2f/400	1.3	P1657
Water	87	79	654				

n-Octane

Alternative names

Reference codes

CAS number	111 65 9	Hazchem code	3YE
UN number	1262	EPA code	

Physical properties

Molecular weight	114	Cubic expansion coeff (per °C × 10^3)	1.2
Empirical formula	C_8H_{18}	Surface tension (@20°C dyn/cm)	21.7
Boiling point (°C)	126	Absolute viscosity (@25°C cP)	0.50
Freezing point (°C)	–57	Refractive index (25°C)	1.395
Specific gravity (20/4)	0.703		

Fire hazards

Flash point (closed cup °C)	13.3	Lower explosive limit (ppm)	10000
Autoignition temperature (°C)	220	Upper explosive limit (ppm)	65000
Electrical conductivity			

Health hazards

IDLH (ppm)	3750	Vapour concentration @21°C ppm	15700
OES-TWA	300	Vapour density (relative to air)	4.1
OES-STEL	375	Vapour pressure @21°C mmHg	12
Odour threshold (ppm)	200	POCP	49

Aqueous effluent

Solubility in water (25°C %w/w)		0.63E–4
Solubility of water in (25°C %w/w)		80E–4
Log_{10} activated carbon partition		
Log_{10} partition in octanol/water (w/w)		
Biological oxygen demand w/w (days)		
Theoretical oxygen demand w/w		

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

Antoine equation	A	6.93142
	B	1358.800
	C	209.855
Cox chart	A	7.14736
	B	1518.9

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)		Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	1.23
Polarity (water 100)	1.2		

Thermal information

Latent heat (cal/mol)	8265
Nett heat of combustion (kcal/gmol)	1213
Specific heat (cal/mol/°C)	59.3
Critical pressure (MN/m^2)	2.49
Critical temperature (K)	568
Latent heat of fusion (cal/mol)	4926
Van der Waals' volume	5.85
Van der Waals' surface area	4.93
Molar volume	163.5

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.0	1x/1/395		
n-Hexane				0.9	6a/613		
n-Heptane	None		12133	1.0	6b/196		
n-Octane	–		–	–	–	–	–
n-Nonane							
n-Decane							
2,2,4-TMP	None		13809	0.9	6b/283		
Cyclohexane	None		11697	1.0	6a/323		
Benzene	0.7	80	10876	1.2	6b/242		
Toluene	None		13027	1.1	6b/261		
Ethylbenzene	88	126	14101	1.2	6b/273		
Xylenes	None		14120	1.2	6b/275		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	37	72	2113	15.4	2c/249		
Ethanol	29	98	4139	21.9	2c/462	6.42	V2/385
n-Propanol	64	88	6514	3.7	2c/576	1.18	V2/585
i-Propanol	50	76	6399	7.0	2b/115	2.55	V2/622
n-Butanol	82	94	8182	4.8	2f/207	1.02	P960
i-Butanol	73	91	8368				
s-Butanol	89	62	8284	26.7	1x/3/1368		
n-Amyl alc.	Azeo			4.1	2f/383	0.24	P1270
i-Amyl alc.	93	98	9869				
Cyclohexanol	None		11727				
1-Octanol							
Ethanediol	97	98	4312				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME	82	123	10002				
EGME	77	93	6592				
EEE	86	97	8461	4.5	2b/302		
EGBE	None			5.0	2b/432	0.93	P3982
Chlorinated							
MDC				2.2	1x/1/393		
Chloroform				1.4	1x/1/393		
Carbon tet.	None		1168a	1.0	6b/234		
1,2-EDC	24	81	3009	2.9	1x/1/393		
1,1,1-TCA							
TCE							
Perk.	8	121	2227				
MCB	None		10531				

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	10	56	5393	6.1	3b/224	0.30	V2/507
MEK	30	77	7384	3.3	3+4/317		
MIBK	87	98	11801	2.1	1x/1/395		
Cyclohexanone							
NMP				14.4	1x/3/1368		
Acetophenone							
Ethers							
Diethyl ether							
DIPE	None		12196				
Dibutyl ether							
MTBE							
1,4-Dioxane	56	92	7552	2.5	3+4/480		
THF				1.5	1x/1/394		
Esters							
Me acetate	3	57	5558				
Et acetate	6	77	7594	2.4	1x/1/394		
i-Propyl acetate	33	88	9302				
n-Butyl acetate	None		11826a				
Cellosolve acetate							
Miscellaneous							
DMF	Azeo			16.5	1x/3/1367		
DMAc							
DMSO							
Sulfolane							
CS_2				1.3	1x/1/393		
Acetic acid	83	95	3204				
Aniline	None		11197	6.2	5/189		
Nitrobenzene				2.5	6b/241		
Morpholine							
Pyridine	75	96	8860	2.9	6b/239		
2-Nitropropane	80	95	6289				
Acetonitrile	34	77	2810	31.3	1x/1/393		
Furfuraldehyde	5	98	8781	8.5	3a/137		
Phenol	None		10936	8.9	2b/382		
Water	75	90	734				

n-Nonane

Alternative names

Reference codes

CAS number		Hazchem code	
UN number	1920	EPA code	

Physical properties

Molecular weight	128	Cubic expansion coeff (per °C × 10^3)	1.1
Empirical formula	C_9H_{20}	Surface tension (@20°C dyn/cm)	22.9
Boiling point (°C)	151	Absolute viscosity (@25°C cP)	0.67
Freezing point (°C)	–53	Refractive index (25°C)	1.403
Specific gravity (20/4)	0.718		

Fire hazards

Flash point (closed cup °C)	31	Lower explosive limit (ppm)	8700
Autoignition temperature (°C)	205	Upper explosive limit (ppm)	29000
Electrical conductivity			

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	5263
OES-TWA	300	Vapour density (relative to air)	4.4
OES-STEL		Vapour pressure @21°C mmHg	4
Odour threshold (ppm)	0.4	POCP	47

Aqueous effluent

Solubility in water (25°C %w/w)	0.2E–4
Solubility of water in (25°C %w/w)	79E–4
Log_{10} activated carbon partition	
Log_{10} partition in octanol/water (w/w)	
Biological oxygen demand w/w (days)	
Theoretical oxygen demand w/w	3.50

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

Antoine equation	A	6.93442
	B	1429.459
	C	201.820
Cox chart	A	7.24534
	B	1662.9

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)		Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)	0.9		

Thermal information

Latent heat (cal/mol)	9037
Nett heat of combustion (kcal/gmol)	1359
Specific heat (cal/mol/°C)	71
Critical pressure (MN/m^2)	2.31
Critical temperature (K)	595
Latent heat of fusion (cal/mol)	3690
Van der Waals' volume	6.52
Van der Waals' surface area	5.48
Molar volume	178.3

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.0	1x/3/1387		
n-Hexane				0.8	1x/3/1387		
n-Heptane				0.8	1x/3/1387		
n-Octane							
n-Nonane	–		–	–	–	–	–
n-Decane							
2,2,4-TMP							
Cyclohexane							
Benzene				1.0	1x/3/1387		
Toluene							
Ethylbenzene	None		14106				
Xylenes	19	144	14118				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	17	64	2119				
Ethanol				6.7	2e/398	6.16	V2/391
n-Propanol	2	97		4.2	2e/505	1.25	V2/586
i-Propanol				9.5	2f/95	2.11	V2/623
n-Butanol	29	116	8203	12.0	2f/209		
i-Butanol							
s-Butanol							
n-Amyl alc.				5.6	1x/3/1387		
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE	50	128	8493				
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				6.4	3b/236		
MEK							
MIBK							
Cyclohexanone							
NMP							
Acetophenone				13.7	1x/3/1387		
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				2.2	3+4/481		
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF				16.1	1x/3/1387		
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	31	113	3230				
Aniline	87	149	11210				
Nitrobenzene							
Morpholine							
Pyridine	10	115	8870	2.4	6b/352		
2-Nitropropane	25	118	6293				
Acetonitrile		80	2812				
Furfuraldehyde							
Phenol							
Water	40	95	789				

n-Decane

Alternative names

Reference codes

CAS number		Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	142	Cubic expansion coeff (per °C × 10^3)	1.06
Empirical formula	$C_{10}H_{22}$	Surface tension (@20°C dyn/cm)	
Boiling point (°C)	174	Absolute viscosity (@25°C cP)	
Freezing point (°C)	–30	Refractive index (25°C)	1.408
Specific gravity (20/4)	0.730		

Fire hazards

Flash point (closed cup °C)	44	Lower explosive limit (ppm)	8000
Autoignition temperature (°C)		Upper explosive limit (ppm)	25000
Electrical conductivity			

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	1980
OES-TWA		Vapour density (relative to air)	4.9
OES-STEL		Vapour pressure @21°C mmHg	1.5
Odour threshold (ppm)		POCP	46.4

Aqueous effluent

Solubility in water (25°C %w/w)	0.02E–4
Solubility of water in (25°C %w/w)	72E–4
Log_{10} activated carbon partition	
Log_{10} partition in octanol/water (w/w)	
Biological oxygen demand w/w (days)	
Theoretical oxygen demand w/w	3.49

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

Antoine equation	A	7.44000
	B	1843.12
	C	230.220
Cox chart	A	7.33946
	B	1801.3

Solvent properties

Solubility parameter	6.7	Kauri butanol value	
Dipole (D)		Evaporation time (ether = 1)	
Dielectric Constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)	0.9		

Thermal information

Latent heat (cal/mol)	
Nett heat of combustion (kcal/gmol)	1504
Specific heat (cal/mol/°C)	
Critical pressure (MN/m^2)	2.11
Critical temperature (K)	617
Latent heat of fusion (cal/mol)	6864
Van der Waals' volume	7.20
Van der Waals' surface area	6.02
Molar volume	195

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.0	1x/4/1410		
n-Hexane				1.0	1x/4/1411		
n-Heptane				1.0	1x/4/1412		
n-Octane				1.0	1x/4/1412		
n-Nonane							
n-Decane	–		–	–	–	–	–
2,2,4-TMP							
Cyclohexane				0.9	1x/4/1411		
Benzene				0.8	6c/574		
Toluene				1.3	1x/4/1411		
Ethylbenzene							
Xylenes							
C_9 Aromatics	75	166	15033				
Tetralin							
Alcohols							
Methanol	None		2126	0.6	2e/193		
Ethanol	None			3.3	2a/508		
n-Propanol	None			5.8	2a/606		
i-Propanol	None			5.1	2b/118		
n-Butanol	92		8213	12.4	2b/236		
i-Butanol							
s-Butanol	None			1.1	2d/285	0.06	V3/133
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol				7.1	2f/542		
Ethanediol	77	161	4434				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	8	123	6628				
EEE							
EGBE							
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB				1.3	6b/392		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5396	1.2	3+4/247		
MEK	None			3.8	3b/396		
MIBK							
Cyclohexanone							
NMP				12.6	1x/4/1410		
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				3.2	1x/4/1410		
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF				15.5	1x/4/1410		
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	20	117	3237	1.1	6c/571		
Aniline	64	167	11230	5.3	5/191		
Nitrobenzene							
Morpholine							
Pyridine	None		8872	1.7	6b/386		
2-Nitropropane							
Acetonitrile		81	2815				
Furfuraldehyde				4.5	3+4/59		
Phenol	65	168	11016				
Water		97	842				

2,2,4-Trimethyl pentane

Alternative names
ISO-Octane, ISOPAR C, 2,2,4-TMP

Reference codes

CAS number	540 84 1	Hazchem code	3YE
UN number		EPA code	

Physical properties

Molecular weight	114	Cubic expansion coeff (per °C × 10^3)	1.00
Empirical formula	C_8H_{18}	Surface tension (@20°C dyn/cm)	18.33
Boiling point (°C)	99	Absolute viscosity (@25°C cP)	0.477
Freezing point (°C)	–107	Refractive index (25°C)	1.389
Specific gravity (20/4)	0.692		

Fire hazards

Flash point (closed cup °C)	–12	Lower explosive limit (ppm)	11000
Autoignition temperature (°C)	418	Upper explosive limit (ppm)	60000
Electrical conductivity			

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	
OES-TWA	400	Vapour density (relative to air)	4.1
OES-STEL		Vapour pressure @21°C mmHg	41
Odour threshold (ppm)		POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		2.2E–4
Solubility of water in (25°C %w/w)		0.011
Log_{10} activated carbon partition		
Log_{10} partition in octanol/water (w/w)		
Biological oxygen demand w/w (days)		
Theoretical oxygen demand w/w		3.51

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

Antoine equation	A	6.80304
	B	1252.59
	C	220.119
Cox chart	A	7.04642
	B	1370.5

Solvent properties

Solubility parameter	7.4	Kauri butanol value	27
Dipole (D)		Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)			

Thermal information

Latent heat (cal/mol)	7396
Nett heat of combustion (kcal/gmol)	1211
Specific heat (cal/mol/°C)	55.6
Critical pressure (MN/m^2)	2.59
Critical temperature (K)	544
Latent heat of fusion (cal/mol)	2157
Van der Waals' volume	5.85
Van der Waals' surface area	5.01
Molar volume	166.1

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane				1.0	1x/1/398		
n-Heptane	None		13809	1.0	6b/197		
n-Octane	None		14715	0.7	6b/283		
n-Nonane							
n-Decane							
2,2,4-TMP	–		–	–	–	–	–
Cyclohexane	None		11699a	1.9	6a/328		
Benzene	2	80	10880	1.4	6b/304		
Toluene	None		13040	1.4	6b/323		
Ethylbenzene	None			1.4	6b/333		
Xylenes							
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	47	59	2114	16.6	2a/250	20.1	V2/139
Ethanol	58	72	4167	29.3	2a/503	31.2	V2/386
n-Propanol	59	85	6524	11.2	2c/500		
i-Propanol	46	77	6419	4.4	2b/116		
n-Butanol							
i-Butanol	73	92	8378				
s-Butanol	66	88	8254	5.2	2b/284		
n-Amyl alc.							
i-Amyl alc.	95	99	9882				
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC				2.1	1x/1/397		
Chloroform				1.5	1x/1/397		
Carbon tet.	None		1168b	1.2	6b/285		
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				2.4	3b/225	0.11	V3/30
MEK	30			3.7	3b/395	0.10	CEH
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane							
THF				1.4	1x/1/398		
Esters							
Me acetate							
Et acetate				3.1	1x/1/398		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2				1.3	1x/1/397		
Acetic acid							
Aniline	None		11196	6.5	6b/318		
Nitrobenzene							
Morpholine							
Pyridine	77	96	8868	7.5	6b/297		
2-Nitropropane	79	95	6292				
Acetonitrile	40	69	2811	31.5	1x/1/397		
Furfuraldehyde	Azeo			13.1	3+4/55		
Phenol	None			17.3	2b/383		
Water	89	79	734a				

Cyclohexane

Alternative names
Hexamethylene, benzene hydride

Reference codes			
CAS number	110 82 7	Hazchem code	3YE
UN number	1145	EPA code	
Physical properties			
Molecular weight	84	Cubic expansion coeff (per °C × 10^3)	1.2
Empirical formula	C_6H_{12}	Surface tension (@20°C dyn/cm)	24.98
Boiling point (°C)	81	Absolute viscosity (@25°C cP)	0.980
Freezing point (°C)	+6.5	Refractive index (25°C)	1.424
Specific gravity (20/4)	0.778		
Fire hazards			
Flash point (closed cup °C)	–17	Lower explosive limit (ppm)	13000
Autoignition temperature (°C)	260	Upper explosive limit (ppm)	84000
Electrical conductivity	7.0E–18		
Health hazards			
IDLH (ppm)	10000	Vapour concentration @21°C ppm	155700
OES-TWA	100	Vapour density (relative to air)	2.9
OES-STEL	300	Vapour pressure @21°C mmHg	78.8
Odour threshold (ppm)	400	POCP	25
Aqueous effluent			
Solubility in water (25°C %w/w)		0.0055	
Solubility of water in (25°C %w/w)		0.01	
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)		+4.15	
Biological oxygen demand w/w (days)		0.6 (5)	
Theoretical oxygen demand w/w		3.43	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	6.85146	
	B	1206.470	
	C	223.136	
Cox chart	A	7.04736	
	B	1295.8	
Solvent properties			
Solubility parameter	8.2	Kauri butanol value	50
Dipole (D)	0.3	Evaporation time (ether = 1)	3.4
Dielectric Constant (20°C)	2.01	Evaporation time (BuAc = 1)	5.6
Polarity (water 100)	0.6		
Thermal information			
Latent heat (cal/mol)	7140		
Nett heat of combustion (kcal/gmol)	874		
Specific heat (cal/mol/°C)	36.4		
Critical pressure (MN/m^2)	4.07		
Critical temperature (K)	553		
Latent heat of fusion (cal/mol)	627		
Van der Waals' volume	4.05		
Van der Waals' surface area	3.24		
Molar volume	108.57		

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.2	6a/119		
n-Hexane	None		11690	4.0	6a/273		
n-Heptane	None		11697	0.9	6a/304		
n-Octane				1.7	6a/323		
n-Nonane							
n-Decane							
2,2,4-TMP	None		11699a	1.0	6a/328		
Cyclohexane	–		–	–	–	–	–
Benzene	50	77	10854	1.4	6a/205	<0.01	V3/278
Toluene	None		11694	1.5	6a/283	<0.01	V3/340
Ethylbenzene				1.7	6a/310		
Xylenes				2.0	6a/311		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	62	54	2079	20.9	2a/239	14.8	P159
Ethanol	70	65	4087	13.0	2a/430	23.0	V2/350
n-Propanol	80	74	6495	10.0	2a/579	6.6	P639
i-Propanol	68	69	6384	12.0	2f/69	8.0	V2/613
n-Butanol	96	80	8146	9.0	2f/179	1.8	P950
i-Butanol	86	78	8338	9.9	2f/317		
s-Butanol	82	76	8234	4.5	2f/234		
n-Amyl alc.	None		9752	16.7	1x/3/1227		
i-Amyl alc.	None		9834				
Cyclohexanol	None		11684				
1-Octanol							
Ethanediol	None		4255				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	85	77	6572	22.1	2b/128		
EEE	None		8430				
EGBE						1.4	P3977
Chlorinated							
MDC							
Chloroform	None		1490				
Carbon tet.	None		1159	1.1	6a/142		
1,2-EDC	50	74	3001	2.6	6a/159		
1,1,1-TCA							
TCE	None		2328	1.5	6a/155		
Perk.							
MCB	None		10515	1.71	6a/202		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	33	53	5378	4.7	3+4/213	1.95	P492
MEK	60	72	7374	2.8	3+4/297	0.13	V3/25
MIBK	None		11685	2.7	3+4/354		
Cyclohexanone				2.7	3+4/337		
NMP				9.4	3b/447		
Acetophenone							
Ethers							
Diethyl ether							
DIPE				1.0	3+4/555		
Dibutyl ether							
MTBE				1.3	1x/3/1227		
1,4-Dioxane	75	80	7540	3.0	3+4/468		
THF				1.6	1x/3/1227		
Esters							
Me acetate	17	55	5341	3.4	5/393		
Et acetate	46	73	7583	2.7	5/506		
i-Propyl acetate	75	79	9296				
n-Butyl acetate				2.1	5/585		
Cellosolve acetate							
Miscellaneous							
DMF				19.2	1x/3/1226		
DMAc				11.2	1x/1/271		
DMSO							
Sulfolane				90.0	1x/3/1227		
CS_2	None		1269	1.1	6a/154		
Acetic acid	9	79	3173	15.6	5/146	12.8	V2/259
Aniline	None		11148	4.7	6a/255	0.2	P1713
Nitrobenzene				9.9	6a/203		
Morpholine							
Pyridine	None		8846	2.8	6a/177		
2-Nitropropane	90	81	6283	6.9	1x/1/270		
Acetonitrile	40	62	2797				
Furfuraldehyde	None		8763	16.7	3+4/45		
Phenol						1.59	P1622
Water	91	70	522				

Benzene

Alternative names
Benzole, benzol, **not** benzine

Reference codes			
CAS number	71 43 2	Hazchem code	3WE
UN number	1114	EPA code	U019
Physical properties			
Molecular weight	78	Cubic expansion coeff (per °C × 10^3)	1.24
Empirical formula	C_6H_6	Surface tension (@20°C dyn/cm)	28.9
Boiling point (°C)	80	Absolute viscosity (@25°C cP)	0.65
Freezing point (°C)	+5.5	Refractive index (25°C)	1.498
Specific gravity (20/4)	0.879		
Fire hazards			
Flash point (closed cup °C)	–11	Lower explosive limit (ppm)	13000
Autoignition temperature (°C)	592	Upper explosive limit (ppm)	71000
Electrical conductivity	4.4E–17		
Health hazards			
IDLH (ppm)	2000	Vapour concentration @21°C ppm	117000
OES-TWA	5	Vapour density (relative to air)	2.8
OES-STEL		Vapour pressure @21°C mmHg	78
Odour threshold (ppm)	300	POCP	19
Aqueous effluent			
Solubility in water (25°C %w/w)		0.18	
Solubility of water in (25°C %w/w)		0.063	
Log_{10} activated carbon partition		3.6	
Log_{10} partition in octanol/water (w/w)		+2.13	
Biological oxygen demand w/w (days)		1.2 (10)	
Theoretical oxygen demand w/w		3.08	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	6.87987	
	B	1196.760	
	C	219.161	
Cox chart	A	7.04500	
	B	1290.9	
Solvent properties			
Solubility parameter	9.2	Kauri butanol value	112
Dipole (D)	0	Evaporation time (ether = 1)	2.6
Dielectric constant (20°C)	2.28	Evaporation time (BuAc = 1)	
Polarity (water 100)	11.1		
Thermal information			
Latent heat (cal/mol)	7340		
Nett heat of combustion (kcal/gmol)	749		
Specific heat (cal/mol/°C)	31		
Critical pressure (MN/m^2)	4.9		
Critical temperature (K)	562		
Latent heat of fusion (cal/mol)	2375		
Van der Waals' volume	3.19		
Van der Waals' surface area	2.40		
Molar volume	89.41		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	None		9741	1.8	6a/118		
n-Hexane	5	68	10861	1.5	6a/535		
n-Heptane	0.7	80	10876	1.7	6b/123		
n-Octane	None		10879	1.2	6b/242		
n-Nonane							
n-Decane	None			1.1	6c/574		
2,2,4-TMP	98	80	10880	1.5	6b/304		
Cyclohexane	50	77	10854	1.5	6a/205		
Benzene	–		–	–	–	–	–
Toluene	None		10871	0.9	7/823		
Ethylbenzene	None		10878a	1.0	7/306		
Xylenes	None			1.0	7/310		
C_9 Aromatics	None		10882a	2.2	7/322		
Tetralin							
Alcohols							
Methanol	61	57	2066	9.7	2a/205	2.3	V2/121
Ethanol	68	68	4073	13.2	2a/399	8.0	P379
n-Propanol	83	77	6491	5.7	2a/556	1.3	P636
i-Propanol	67	72	6375	6.9	2f/65	0.86	V2/595
n-Butanol	None		8136	4.3	2f/169	0.19	V3/118
i-Butanol	92	79	8333	116.0	2f/316	0.24	V3/142
s-Butanol	85	79	8232	3.6	2f/227	0.33	V3/129
n-Amyl alc.	None		9748			0.15	P1268
i-Amyl alc.	None		9821				
Cyclohexanol	None		10856				
1-Octanol							
Ethanediol	None		4239				
DEG	None		8520				
1,2-Propanediol	None		6654				
Glycol ethers							
PGME							
EGME	None		6567	5.7	2b/127		
EEE	None		8425				
EGBE						1.42	P3978
Chlorinated							
MDC				0.9	1x/1/225		
Chloroform	None		1486	0.9	7/80		
Carbon tet.	None		1154	1.1	7/7		
1,2-EDC	82	80	2999	1.0	7/142		
1,1,1-TCA				1.0	7/121		
TCE	None		2326	1.0	7/114		
Perk.	None			1.3	7/112		
MCB	None		10509	1.0	7/243		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5374	1.9	3+4/195	0.43	P497
MEK	55	78	7369	1.3	3+4/284		
MIBK	None		10857	1.1	3+4/351		
Cyclohexanone				0.7	3b/503		
NMP				1.0	3b/441		
Acetophenone						0.001	P2745
Ethers							
Diethyl ether	None		8293	0.7	3+4/516		
DIPE	None		10863	1.2	3+4/553		
Dibutyl ether							
MTBE							
1,4-Dioxane	88	12	7537	1.1	3+4/465	0.24	V3/72
THF				0.8	1x/3/1183	0.06	V4/238
Esters							
Me acetate	0.3	43	5537	1.3	5/375	0.08	P518
Et acetate	6	77	7580	3.7	5/502	0.02	P863
i-Propyl acetate	None		9294				
n-Butyl acetate	None		10859	0.9	5/583	<0.01	V3/279
Cellosolve acetate							
Miscellaneous							
DMF	None		5863	4.6	1x/1/226	3.33	V2/542
DMAc				3.4	1x/1/227		
DMSO	None		4184	3.3	7/169		
Sulfolane				3.8	7/191	0.53	V3/88
CS_2	None		1265	1.3	7/100		
Acetic acid	98	80	3163	5.1	5/127	21.0	P301
Aniline	None		10850	1.5	7/263	0.12	P1716
Nitrobenzene	None		10703	1.5	7/253		
Morpholine						2.49	V3/105
Pyridine	None		8841	1.2	7/220	0.09	P1104
2-Nitropropane	None		6281	2.2	7/186		
Acetonitrile	66	73	2795	3.0	7/124	0.03	V2/182
Furfuraldehyde	None		8760	1.8	3+4/44	0.05	V3/190
Phenol	None			4.8	2b/359	0.08	V3/265
Water	91	69	486				

Toluene

Alternative names
Toluol, methylbenzene, methylbenzol

Reference codes			
CAS number	108 88 3	Hazchem code	3YE
UN number	1294	EPA code	U220
Physical properties			
Molecular weight	92	Cubic expansion coeff (per °C × 10^3)	1.1
Empirical formula	C_7H_8	Surface tension (@20°C dyn/cm)	28.5
Boiling point (°C)	110.6	Absolute viscosity (@25°C cP)	0.59
Freezing point (°C)	–95	Refractive index (25°C)	1.494
Specific gravity (20/4)	0.867		
Fire hazards			
Flash point (closed cup °C)	4	Lower explosive limit (ppm)	12700
Autoignition temperature (°C)	480	Upper explosive limit (ppm)	70000
Electrical conductivity	8.0E–16		
Health hazards			
IDLH (ppm)	2000	Vapour concentration @21°C ppm	31000
OES-TWA	50	Vapour density (relative to air)	3.2
OES-STEL	150	Vapour Pressure @21°C mmHg	23.2
Odour threshold (ppm)	40	POCP	56

Aqueous effluent	
Solubility in water (25°C %w/w)	0.052
Solubility of water in (25°C %w/w)	0.033
Log_{10} activated carbon partition	2.9
Log_{10} partition in octanol/water (w/w)	+2.69
Biological oxygen demand w/w (days)	1.19 (5)
Theoretical oxygen demand w/w	3.13

Vapour pressure equation constants (Log_{10}, mmHg)		
Antoine equation	A	6.95087
	B	1342.31
	C	219.187
Cox chart	A	7.12773
	B	1448.2

Solvent properties			
Solubility parameter	8.9	Kauri butanol value	105
Dipole (D)	0.4	Evaporation time (ether = 1)	6.1
Dielectric Constant (20°C)	2.38	Evaporation time (BuAc = 1)	2.0
Polarity (water 100)	9.9		

Thermal information	
Latent heat (cal/mol)	7985
Nett heat of combustion (kcal/gmol)	892
Specific heat (cal/mol/°C)	41.0
Critical pressure (MN/m^2)	4.22
Critical temperature (K)	591.8
Latent heat of fusion (cal/mol)	1580
Van der Waals' volume	3.92
Van der Waals' surface area	2.97
Molar volume	106.85

Solute	Azeotrope X% w/w	Azeotrope °C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.3	6c/160		
n-Hexane	None		12131	1.4	6a/591		
n-Heptane	None		13027	1.2	6b/169		
n-Octane	None		13041	1.3	6b/261		
n-Nonane							
n-Decane							
2,2,4-TMP	None		13043	1.4	6b/323		
Cyclohexane	None		11694	1.2	6a/283		
Benzene	None		10871	1.0	7/283		
Toluene	–		–	–	–	–	–
Ethylbenzene	None		13029	1.1	7/443		
Xylenes	None		13030	0.83	7/444		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	31	64	2098	6.3	2a/268	20.8	V2/135
Ethanol	32	77	4120	5.3	2a/477	11.6	V2/372
n-Propanol	51	93	6512	4.3	2a/592	1.05	V2/580
i-Propanol	31	81	6397	3.9	2f/78	1.16	V2/619
n-Butanol	68	106	8170	10.3	2f/190	0.17	CEH
i-Butanol	55	101	8361	3.8	2b/289		
s-Butanol	45	95	8246	3.3	2d/276	0.20	V3/130
n-Amyl alc.	None		9760				
i-Amyl alc.	90	110	9852				
Cyclohexanol	None		11720				
1-Octanol							
Ethanediol	93	110	4285				
DEG	None		8531	45.9	2f/341		
1,2-Propanediol	98	110	6658				
Glycol ethers							
PGME	None		9978				
EGME	74	106	6586				
EEE	89	110	8450	3.9	2f/337		
EGBE	None			1.4	2f/440	0.78	P3980
Chlorinated							
MDC				0.9	1x/3/317		
Chloroform	None		1498	1.2	7/352		
Carbon tet.	None		1166	1.0	7/332		
1,2-EDC	None		3006	1.0	7/380		
1,1,1-TCA							
TCE				0.9	7/370		
Perk.	None		2220				
MCB	None		10524	1.0	7/416		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5391	1.8	3+4/236	0.40	P501
MEK	None		7382	1.4	3+4/308		
MIBK	97	111	11799	1.2	3+4/356		
Cyclohexanone				1.4	3+4/339		
NMP				0.3	3b/456		
Acetophenone							
Ethers							
Diethyl ether	None		8304				
DIPE				1.2	3+4/558		
Dibutyl ether							
MTBE							
1,4-Dioxane	20	102	7550	1.3	3+4/375		
THF							
Esters							
Me acetate							
Et acetate	None		7591	1.2	5/516		
i-Propyl acetate	None		9300				
n-Butyl acetate	None		11825	1.1	5/586		
Cellosolve acetate	None		11913				
Miscellaneous							
DMF	None		5893a	1.9	7/390	2.22	V4/223
DMAc							
DMSO	None			8.3	7/386		
Sulfolane				140.4	7/399		
CS_2	None		1276	1.1	7/361		
Acetic acid	72	101	3194	9.4	5/159	2.97	V4/190
Aniline	None		11167	1.7	7/426	0.03	P1719
Nitrobenzene	None		10718	1.9	7/422		
Morpholine							
Pyridine	68	108	8858	1.8	7/406	0.14	P1109
2-Nitropropane	82	110	6285				
Acetonitrile	24	81	2801	3.8	7/373	0.07	V2/191
Furfuraldehyde	None		8776	2.6	3a/135	0.03	V4/258
Phenol	None		10920	2.4	2f/393	0.12	P1644
Water	80	85		610			

Ethylbenzene

Alternative names
Phenyl ethane

Reference codes

CAS number	100 41 4	Hazchem code	3YE
UN number	1175	EPA code	Z048

Physical properties

Molecular weight	106	Cubic expansion coeff (per °C × 10^3)	1.03
Empirical formula	C_8H_{10}	Surface tension (@20°C dyn/cm)	29.2
Boiling point (°C)	136	Absolute viscosity (@25°C cP)	0.72
Freezing point (°C)	–94	Refractive index (25°C)	1.493
Specific gravity (20/4)	0.867		

Fire hazards

Flash point (closed cup °C)	15	Lower explosive limit (ppm)	10000
Autoignition temperature (°C)	435	Upper explosive limit (ppm)	67000
Electrical conductivity			

Health hazards

IDLH (ppm)	2000	Vapour concentration @21°C ppm	9960
OES-TWA	100	Vapour density (relative to air)	3.7
OES-STEL	125	Vapour pressure @21°C mmHg	8.0
Odour threshold (ppm)	125	POCP	59

Aqueous effluent

Solubility in water (25°C %w/w)	0.020
Solubility of water in (25°C %w/w)	0.033
Log_{10} activated carbon partition	3.1
Log_{10} partition in octanol/water (w/w)	+2.76
Biological oxygen demand w/w (days)	0.028 (5)
Theoretical oxygen demand w/w	3.17

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

Antoine equation	A	6.96580
	B	1429.550
	C	213.767
Cox chart	A	7.19691
	B	1579.7

Solvent properties

Solubility Parameter	8.9	Kauri butanol value	
Dipole (D)	0.4	Evaporation time (ether = 1)	8.8
Dielectric constant (20°C)	2.41	Evaporation time (BuAc = 1)	0.84
Polarity (water 100)			

Thermal information

Latent heat (cal/mol)	8491
Nett heat of combustion (kcal/gmol)	1038
Specific heat (cal/mol/°C)	43
Critical pressure (MN/m^2)	3.74
Critical temperature (K)	617
Latent heat of fusion (cal/mol)	
Van der Waals' volume	4.60
Van der Waals' surface area	3.51
Molar volume	123.1

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane							
n-Heptane	None		13807	1.7	6c/489		
n-Octane	12	126	14101	1.2	6b/273		
n-Nonane	None		14106				
n-Decane							
2,2,4-TMP	None			1.5	6b/333		
Cyclohexane				1.2	6a/310		
Benzene	None		10878a	1.0	7/306		
Toluene	None		13029	1.0	7/443		
Ethylbenzene	–		–	–	–	–	–
Xylenes	None		14098				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	None		2106	6.5	2c/245		
Ethanol	None		4144	6.1	2c/460		
n-Propanol	9	97	6517	3.3	2a/601		
i-Propanol	None		6402	2.0	2d/95	2.0	V2/621
n-Butanol	33	115	8185	2.7	2b/228		
i-Butanol	20	107	8371				
s-Butanol	None		8251				
n-Amyl alc.	60	130	9765				
i-Amyl alc.	51	126	9871				
Cyclohexanol							
1-Octanol							
Ethanediol	87	133	4321				
DEG	Azeo		8545				
1,2-Propanediol							
Glycol ethers							
PGME	80	135	9991				
EGME	49	117	6596	3.1	2b/132		
EEE	57	126	8463	2.9	2b/299	2.0	V3/158
EGBE	4	140				0.85	P3977
Chlorinated							
MDC							
Chloroform							
Carbon tet.	None		1167a	0.9	7/464		
1,2-EDC				0.7	7/466		
1,1,1-TCA							
TCE							
Perk.	None		2225				
MCB				1.0	7/469		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None			2.1	3b/217		
MEK	None			1.4	3+4/316		
MIBK	None		11802				
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE				1.1	3+4/563		
Dibutyl ether	None		14102				
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate				0.9	5/540		
i-Propyl acetate							
n-Butyl acetate	None		11828				
Cellosolve acetate	None		12007				
Miscellaneous							
DMF	85	134					
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	34	115	3206	5.0	5/178		
Aniline	None		11183	2.0	7/474		
Nitrobenzene				1.6	7/470		
Morpholine				1.5	3+4/482		
Pyridine	None		8861				
2-Nitropropane	8	120	6290				
Acetonitrile	None		2804	2.5	7/465		
Furfuraldehyde	95	132	8783	3.0	3+4/51		
Phenol	None		10943			0.07	V4/268
Water	67	92	676				

Xylenes (mixed isomers)

Alternative names
Dimethyl benzenes, xylol

Reference codes			
CAS number	1330 20 7	Hazchem code	3Y
UN number	1307	EPA code	U239
*Physical properties**			
Molecular weight	106	Cubic expansion coeff (per °C x 10^3)	1.0
Empirical formula	C_8H_{10}	Surface tension (@20°C dyn/cm)	28.6
Boiling point (°C)	136*	Absolute viscosity (@25°C cP)	0.7*
Freezing point (°C)		Refractive index (25°C)	1.496
Specific gravity (20/4)	0.870		
Fire hazards			
Flash point (closed cup °C)	23*	Lower explosive limit (ppm)	11400
Autoignition temperature (°C)	480	Upper explosive limit (ppm)	70000
Electrical conductivity	8.0E–16		
Health hazards			
IDLH (ppm)	10000	Vapour concentration @21°C ppm	9180
OES-TWA	100	Vapour density (relative to air)	3.7
OES-STEL	150	Vapour pressure @ 21°C mmHg	7.0
Odour threshold (ppm)	1.0	POCP	85*

Aqueous effluent	
Solubility in water (25°C %w/w)	0.02
Solubility of water in (25°C %w/w)	0.05
Log_{10} activated carbon partition	4.3
Log_{10} partition in octanol/water (w/w)	3.0
Biological oxygen demand w/w (days)	0.1 (5)
Theoretical oxygen demand w/w	3.17

*Vapour pressure equation constants (Log_{10}, mmHg)**		
Antoine equation	A	6.99053
	B	1453.43
	C	215.310
Cox chart	A	7.20807
	B	1601.1

Solvent properties			
Solubility parameter	8.9	Kauri butanol value	98
Dipole (D)	1.3	Evaporation time (ether = 1)	13.5
Dielectric constant (20°C)	2.3	Evaporation time (BuAc = 1)	0.76
Polarity (water 100)	7.4		

Thermal information	
Latent heat (cal/mol)	8692
Nett heat of combustion (kcal/gmol)	1035
Specific heat (cal/mol/°C)	42
Critical pressure (MN/m^2)	3.55
Critical temperature (K)	623
Latent heat of fusion (cal/mol)	3180
Van der Waals' volume	4.66
Van der Waals' surface area	3.54
Molar volume	121.84

*Typical mixture of isomers

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				1.5	1x/1/369		
n-Hexane	None			1.2	6a/605		
n-Heptane	None		13808	1.4	6c/497		
n-Octane	None		14120	1.3	6b/275		
n-Nonane	81	144	14118				
n-Decane							
2,2,4-TMP							
Cyclohexane				1.5	6a/311		
Benzene	None			1.0	7/310		
Toluene	None		13030	1.1	7/444		
Ethylbenzene	None		14098				
Xylenes	–		–	–	–	–	–
C_9 Aromatics	None						
Tetralin							
Alcohols							
Methanol	None		2108	6.6	2c/247		
Ethanol	None		4146	5.3	2a/500	3.08	V2/379
n-Propanol	7	97	6519	3.3	2c/575		
i-Propanol	None		6402	2.6	2d/229		
n-Butanol	27	115	8186	3.1	2b/229		
i-Butanol	12	108		2.6	2b/292		
s-Butanol	None		8252	2.7	2d/282		
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol	90	140	11730				
1-Octanol	None	11	4113	6.3	2f/536		
Ethanediol	93	135	4323				
DEG	Azeo						
1,2-Propanediol							
Glycol ethers							
PGME	73	137	9994				
EGME	45	120	6598	4.0	2b/134		
EEE	50	128	8465	4.2	2f/416		
EGBE	4	144	12235			0.56	P3979
Chlorinated							
MDC				0.85	1x/1/369		
Chloroform							
Carbon tet.				0.9	7/480		
1,2-EDC				1.1	7/490		
1,1,1-TCA							
TCE							
Perk.	None		1167c				
MCB				0.9	7/508		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None			2.4	3b/222	0.29	,V2/506
MEK				1.2	3b/382		
MIBK	None			1.3	3b/553		
Cyclohexanone				1.2	3b/511		
NMP				1.9	3b/462		
Acetophenone							
Ethers							
Diethyl ether				1.1	1x/3/1348		
DIPE							
Dibutyl ether	22	142	14117				
MTBE							
1,4-Dioxane				1.3	1x/3/1350		
THF							
Esters							
Me acetate							
Et acetate	None		7594	1.6	5/541		
i-Propyl acetate							
n-Butyl acetate	None		11829				
Cellosolve acetate	None		12009				
Miscellaneous							
DMF	80	136	5894	2.5	7/481		
DMAc							
DMSO							
Sulfolane							
CS_2				1.1	1x/1/369		
Acetic acid	22	116	3208	3.8	5/181	14.1	P310
Aniline	None		11185			0.11	P1718
Nitrobenzene							
Morpholine							
Pyridine				1.4	7/482	0.08	P1108
2-Nitropropane							
Acetonitrile	None		2805	5.1	1x/1/369	0.38	V2/193
Furfuraldehyde	90	139	8785	2.9	3+4/52		
Phenol	None		10944			0.12	P1642
Water	63	93	677				

C_9 Aromatics

Alternative names

Reference codes

CAS number		Hazchem code	
UN number	2325	EPA code	

Physical properties

Molecular weight	120	Cubic expansion coeff (per °C × 10^3)	0.89
Empirical formula	C_9H_{12}	Surface tension (@20°C dyn/cm)	28
Boiling point (°C)	152*	Absolute viscosity (@25°C cP)	1.153
Freezing point (°C)		Refractive index (25°C)	
Specific gravity (20/4)	0.876		

Fire hazards

Flash point (closed cup °C)	55	Lower explosive limit (ppm)	9000
Autoignition temperature (°C)	425	Upper explosive limit (ppm)	65000
Electrical conductivity			

Health hazards

IDLH (ppm)	8000	Vapour concentration @21°C ppm	5200
OES-TWA	25	Vapour density (relative to air)	4.2
OES-STEL	75	Vapour pressure @21°C mmHg	4
Odour threshold (ppm)	0.4	POCP	84*

Aqueous effluent

Solubility in water (25°C %w/w)		0.0058*
Solubility of water in (25°C %w/w)		0.035*
Log_{10} activated carbon partition		
Log_{10} partition in octanol/water (w/w)		
Biological oxygen demand w/w (days)		
Theoretical oxygen demand w/w		3.20

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

Antoine equation	A	7.0764
	B	1571.0
	C	209.7
Cox chart	A	7.25282
	B	1670.2

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)		Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)	7.1		

*Thermal information**

Latent heat (cal/mol)	8952
Nett heat of combustion (kcal/gmol)	1179
Specific heat (cal/mol/°C)	48
Critical pressure (MN/m^2)	3.21
Critical temperature (K)	631
Latent heat of fusion (cal/mol)	1680
Van der Waals' volume	5.30
Van der Waals' surface area	4.04
Molar volume	139

*Typical mixture of isomers

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane							
n-Heptane							
n-Octane							
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane							
Benzene	None		10882a	1.1	7/322		
Toluene							
Ethylbenzene							
Xylenes							
C_9 Aromatics	–	–	–	–	–	–	
Tetralin							
Alcohols							
Methanol	None		2116				
Ethanol	None		4173				
n-Propanol	None		6529				
i-Propanol	None		6422	2.6	2d/97		
n-Butanol	None		8201				
i-Butanol	None		8382				
s-Butanol				2.2	2f/241		
n-Amyl alc.							
i-Amyl alc.	?	?	9886				
Cyclohexanol	50	156	11750				
1-Octanol	None		14729				
Ethanediol	85	153	4372				
DEG							
1,2-Propanediol							
Glycol ethers							
PGME	30	148	10008				
EGME	15	122	6618	3.3	2d/131		
EEE	10	134	8484				
EGBE	20	160	12252				
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB	None		10566				

Hydrocarbons

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^∞	Reference	Partition coefficient	Reference
Ketones							
Acetone						0.33	V2/508
MEK							
MIBK							
Cyclohexanone	?	152	11374				
NMP				2.8	3b/463		
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate	25	155	12024				
Miscellaneous							
DMF	Azeo						
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	None		3225				
Aniline	90	167	11205				
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde	40	152	8805				
Phenol	20	158	10971	2.8	2b/385	0.02	V3/301
Water	50	95	767	52.1	1b/286		

Although individual C_9 aromatics can be obtained commercially the mixture used as a solvent usually contains a mixture of up to eight isomers with atmospheric boiling points in the range of 152–176°C. In many cases some isomers form azeotropes with other solvents while others do not. If any azeotropes are reported they are included in the above table.

Tetralin

Alternative names
Tetrahydronaphthalene, tetranap

Reference codes

CAS number	119 64 2	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	132	Cubic expansion coeff (per °C x 10^3)	1.0
Empirical formula	$C_{10}H_{12}$	Surface tension (@20°C dyn/cm)	35.5
Boiling point (°C)	205	Absolute viscosity (@25°C cP)	2.0
Freezing point (°C)	–31	Refractive index (25°C)	1.539
Specific gravity (20/4)	0.974		

Fire hazards

Flash point (closed cup °C)	74	Lower explosive limit (ppm)	8000
Autoignition temperature (°C)	225	Upper explosive limit (ppm)	50000
Electrical conductivity			

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	526
OES-TWA	25	Vapour density (relative to air)	4.6
OES-STEL		Vapour pressure @21°C mmHg	0.4
Odour threshold (ppm)		POCP	

Aqueous effluent

Solubility in water (25°C %w/w)		
Solubility of water in (25°C %w/w)		
Log_{10} activated carbon partition		4.8
Log_{10} partition in octanol/water (w/w)		
Biological oxygen demand w/w (days)		**0 (5)**
Theoretical oxygen demand w/w		**3.15**

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

Antoine equation	A	
	B	
	C	
Cox chart	A	7.52287
	B	2019.3

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)	0	Evaporation time (ether = 1)	200
Dielectric constant (20°C)	2.77	Evaporation time (BuAc = 1)	
Polarity (water 100)	9.3		

Thermal information

Latent heat (cal/mol)	10098
Nett heat of combustion (kcal/gmol)	1289
Specific heat (cal/mol/°C)	0.53
Critical pressure (MN/m^2)	3.65
Critical temperature (K)	447
Latent heat of fusion (cal/mol)	2978
Van der Waals' volume	
Van der Waals' surface area	
Molar volume	136

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ°	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane				1.9	1x/4/1398		
n-Heptane				1.9	1x/4/1398		
n-Octane							
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane				1.4	1x/4/1398		
Benzene				1.0	1x/4/1398		
Toluene							
Ethylbenzene							
Xylenes							
C_9 Aromatics							
Tetralin	–		–	–	–	–	–
Alcohols							
Methanol							
Ethanol							
n-Propanol							
i-Propanol							
n-Butanol				2.2	2b/235		
i-Butanol							
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol	13	194		2.1	2f/541		
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							
MEK							
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid						4.6	V2/310
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde							
Phenol							
Water	20	99	806				