Section 5

Ketones

Acetone

Alternative names
Propan-2-one, dimethyl ketone

Reference codes			
CAS number	67 64 1	Hazchem code	2YE
UN number	1090	EPA code	U002
Physical properties			
Molecular weight	58	Cubic expansion coeff (per °C × 10^3)	1.4
Empirical formula	$C_3H_6O_1$	Surface tension (@20°C dyn/cm)	23.3
Boiling point (°C)	56	Absolute viscosity (@25°C cP)	0.33
Freezing point (°C)	–95	Refractive index (25°C)	1.357
Specific gravity (20/4)	0.790		
Fire hazards			
Flash point (closed cup °C)	–18	Lower explosive limit (ppm)	26000
Autoignition temperature (°C)	465	Upper explosive limit (ppm)	128000
Electrical conductivity	5E–9		
Health hazards			
IDLH (ppm)	20000	Vapour concentration @21°C ppm	342800
OES-TWA	750	Vapour density (relative to air)	2.0
OES-STEL	1500	Vapour pressure @21°C mmHg	194
Odour threshold (ppm)	300	POCP	17.8
Aqueous effluent			
Solubility in water (25°C %w/w)		Total	
Solubility of water in (25°C %w/w)		Total	
Log_{10} activated carbon partition		1.74	
Log_{10} partition in octanol/water (w/w)		–0.24	
Biological oxygen demand w/w (days)			1.22 (5)
Theoretical oxygen demand w/w		2.21	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.11714	
	B	1210.596	
	C	229.664	
Cox chart	A	7.18990	
	B	1232.4	
Solvent properties			
Solubility parameter	10.0	Kauri butanol value	
Dipole (D)	2.9	Evaporation time (ether = 1)	1.8
Dielectric constant (20°C)	20.6	Evaporation time (BuAc = 1)	5.6
Polarity (water 100)	35.5		
Thermal information			
Latent heat (cal/mol)	7076		
Nett heat of combustion (kcal/gmol)	395		
Specific heat (cal/mol/°C)	30		
Critical pressure (MN/m^2)	4.8		
Critical temperature (K)	508		
Latent heat of fusion (cal/mol)	1358		
Van der Waals' volume	2.57		
Van der Waals' surface area	2.34		
Molar volume	73.4		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	21	32	5368	5.8	3+4/190		
n-Hexane	59	50	5385	5.1	3+4/225		
n-Heptane	90	56	5393	5.5	3+4/242		
n-Octane	None		5395	8.4	3b/224		
n-Nonane	None			6.2	3b/236		
n-Decane	None		5396	6.7	3+4/247		
2,2,4-TMP	None			8.2	3b/225		
Cyclohexane	67	53	5378	4.3	3+4/213		
Benzene	None		5374	1.4	3+4/195		
Toluene	None		5391	1.6	3+4/236		
Ethylbenzene	None			2.1	3b/217		
Xylenes	None			2.6	3b/222		
C_9 Aromatics	None			1.6	3b/233		
Tetralin							
Alcohols							
Methanol	88	55	1963	1.8	2a/68		
Ethanol	None		3965	1.7	2a/321		
n-Propanol	None		5320				
i-Propanol	None		5319	2.4	2b/43		
n-Butanol	None		5344	1.6	2b/140		
i-Butanol	None		5347	1.2	2f/304		
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol	None			4.6	2d/510		
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME				2.9	2d/113		
EEE	None			1.0	2f/332		
EGBE							
Chlorinated							
MDC	None		1553	0.7	3b/27		
Chloroform	22	64	1443	0.6	3+4/90		
Carbon tet.	89	56	1108	2.3	3+4/80		
1,2-EDC	None		2966	1.0	3+4/144		
1,1,1-TCA							
TCE	None		2289	2.7	3b/51		
Perk.	None		2168	3.7	3b/49		
MCB	None		5372	1.6	3+4/192		

Ketones

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	–		–	–	–	–	–
MEK	None		5330	0.9	3+4/173		
MIBK	None		5382	1.1	3b/196		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	None		5346	1.4	3+4/177		
DIPE	61	54	5386				
Dibutyl ether							
MTBE							
1,4-Dioxane	None		5333	1.4	1x/3/991		
THF							
Esters							
Me acetate	50	55	5310	1.3	3+4/159		
Et acetate	None		5334	1.2	3+4/176		
i-Propyl acetate	None		5365				
n-Butyl acetate	None		5383	1.1	3b/197		
Cellosolve acetate							
Miscellaneous							
DMF	None			3.1	3+4/164		
DMAc							
DMSO	None			1.2	3b/80		
Sulfolane							
CS_2	33	39	1194	3.6	3+4/132		
Acetic acid	None		3101	1.4	3+4/148		
Aniline	None			0.9	3b/183		
Nitrobenzene							
Morpholine							
Pyridine	None		5353	2.1	3+4/181		
2-Nitropropane							
Acetonitrile	None		2762	1.0	3+4/143		
Furfuraldehyde							
Phenol	None		5375				
Water	None		269	5.3	1x/3/993		

Methyl ethyl ketone

Alternative names
MEK, butan-2-one

Reference codes

CAS number	78 93 3	Hazchem code	2YE
UN number	1193	EPA code	U159

Physical properties

Molecular weight	72	Cubic expansion coeff (per °C × 10^3)	1.3
Empirical formula	$C_4H_8O_1$	Surface tension (@20°C dyn/cm)	24.6
Boiling point (°C)	80	Absolute viscosity (@25°C cP)	0.41
Freezing point (°C)	–87	Refractive index (25°C)	1.377
Specific gravity (20/4)	0.805		

Fire hazards

Flash point (closed cup °C)	–6	Lower explosive limit (ppm)	18000
Autoignition temperature (°C)	485	Upper explosive limit (ppm)	100000
Electrical conductivity	3.6E–9		

Health hazards

IDLH (ppm)	3000	Vapour concentration @21°C ppm	112000
OES-TWA	200	Vapour density (relative to air)	2.50
OES-STEL	300	Vapour pressure @21°C mmHg	75.3
Odour threshold (ppm)	30	POCP	42.3

Aqueous effluent

Solubility in water (25°C %w/w)	26
Solubility of water in (25°C %w/w)	12.0
Log_{10} activated carbon partition	2.25
Log_{10} partition in octanol/water (w/w)	+0.29
Biological oxygen demand w/w (days)	2.14 (5)
Theoretical oxygen demand w/w	2.44

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

Antoine equation	A	7.06356
	B	1261.340
	C	221.969
Cox chart	A	7.22242
	B	1345.9

Solvent properties

Solubility parameter	9.3	Kauri butanol value	
Dipole (D)	2.8	Evaporation time (ether = 1)	2.5
Dielectric constant (20°C)	18.5	Evaporation time (BuAc = 1)	4.6
Polarity (water 100)	32.7		

Thermal information

Latent heat (cal/mol)	7848
Nett heat of combustion (kcal/gmol)	540
Specific heat (cal/mol/°C)	38
Critical pressure (MN/m^2)	4.16
Critical temperature (K)	535
Latent heat of fusion (cal/mol)	1790
Van der Waals' volume	3.25
Van der Waals' surface area	2.88
Molar volume	89.44

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				3.4	1x/3/1044		
n-Hexane	29	64	7376	2.9	3+4/302		
n-Heptane	70	77	7384	3.2	3+4/311	0.12	CEH
n-Octane				6.0	3+4/317		
n-Nonane							
n-Decane	None			5.0	3b/396		
2,2,4-TMP	None			4.3	3b/395		
Cyclohexane	40	72	7374	3.3	3+4/297		
Benzene	45	78	7369	1.2	3+4/284		
Toluene	None		7382	1.6	3+4/308		
Ethylbenzene	None			1.9	3+4/316		
Xylenes				1.3	3b/382		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	30	64	1993	2.0	2a/133		
Ethanol	61	74	4005	2.3	2a/343		
n-Propanol	None		6445	1.6	2c/496	0.25	V3/225
i-Propanol	68	78	6335	1.6	2b/54		
n-Butanol	None		7357	0.9	2f/144	0.22	V3/17
i-Butanol	None		7360				
s-Butanol	None		7358	1.3	2b/239		
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol						8.16	V2/418
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME				1.8	2b/122		
EEE				1.6	2f/334		
EGBE	None			2.4	2b/430	0.08	CEH
Chlorinated							
MDC	None		1564	0.6	3+4//261		
Chloroform	83	80	1460	0.5	3+4/260		
Carbon tet.	29	74	1121	1.5	3+4/259		
1,2-EDC	24		2977	0.7	3b/271		
1,1,1-TCA							
TCE	None		2299	1.1	3+4/264		
Perk.				2.5	3b/265		
MCB	None			1.5	3+4/283		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5330	0.9	3+4/173	0.30	V4/215
MEK	–		–	–	–	–	–
MIBK				1.0	3+4/300		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE				1.5	3b/357		
Dibutyl ether							
MTBE							
1,4-Dioxane	None		7344	1.2	1x/3/1044		
THF							
Esters							
Me acetate	None		5519	1.0	3+4/271		
Et acetate	12	77	7345	1.1	3+4/278		
i-Propyl acetate	None		7366				
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF				1.4	3b/289		
DMAc							
DMSO							
Sulfolane							
CS_2	16	46	1216	3.0	1x/1/97		
Acetic acid	None		3117	1.6	3+4/269	0.21	P326
Aniline							
Nitrobenzene				1.5	3b/316		
Morpholine							
Pyridine				1.1	1x/1/98		
2-Nitropropane	None		6272				
Acetonitrile	73			1.2	3b/268		
Furfuraldehyde							
Phenol	None		7370	0.1	2b/358		
Water	89	73	338	6.9	1x/1/99		

Methyl isobutyl ketone

Alternative names
4-Methyl-2-pentanone, MIBK

Reference codes			
CAS number	108 10 1	Hazchem code	
UN number	1245	EPA code	U161
Physical properties			
Molecular weight	100	Cubic expansion coeff (per °C × 10^3)	0.94
Empirical formula	$C_6H_{12}O_1$	Surface tension (@20°C dyn/cm)	23.6
Boiling point (°C)	116	Absolute viscosity (@25°C cP)	0.61
Freezing point (°C)	–84	Refractive index (25°C)	1.394
Specific gravity (20/4)	0.801		
Fire hazards			
Flash point (closed cup °C)	13	Lower explosive limit (ppm)	14000
Autoignition temperature (°C)	459	Upper explosive limit (ppm)	75000
Electrical conductivity	5E–8		
Health hazards			
IDLH (ppm)		Vapour concentration @21°C ppm	21700
OES-TWA	50	Vapour density (relative to air)	3.47
OES-STEL		Vapour pressure @21°C mmHg	16.5
Odour threshold (ppm)	8	POCP	63.3
Aqueous effluent			
Solubility in water (25°C %w/w)		1.7	
Solubility of water in (25°C %w/w)		1.9	
Log_{10} activated carbon partition		3.05	
Log_{10} partition in octanol/water (w/w)			
Biological oxygen demand w/w (days)		2.06	
Theoretical oxygen demand w/w		2.2	

Vapour pressure equation constants (Log_{10}, mmHg)		
Antoine equation	A	6.67272
	B	1168.408
	C	191.944
Cox chart	A	7.27155
	B	1519.2

Solvent properties			
Solubility parameter	8.4	Kauri butanol value	
Dipole (D)	2.81	Evaporation time (ether = 1)	5.6
Dielectric constant (20°C)	13.1	Evaporation time (BuAc = 1)	1.4
Polarity (water 100)	27		
Thermal information			
Latent heat (cal/mol)	8500		
Nett heat of combustion (kcal/gmol)	672		
Specific heat (cal/mol/°C)	46		
Critical pressure (MN/m^2)	3.27		
Critical temperature (K)	571.5		
Latent heat of fusion (cal/mol)			
Van der Waals' volume	4.60		
Van der Waals' surface area	3.95		
Molar volume	125.8		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				2.3	1x/3/1233		
n-Hexane				2.5	1x/1/273		
n-Heptane	13	98	11801	2.1	3b/550		
n-Octane	65	113	11805	2.0	1x/1/273		
n-Nonane							
n-Decane							
2,2,4-TMP				1.9	1x/1/373		
Cyclohexane	None		11685	1.2	3+4/354		
Benzene	None		10857	1.0	3+4/351		
Toluene	3	111	11799	1.1	3+4/356		
Ethylbenzene	None		11802				
Xylenes	None			1.6	3b/553		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	None		2084	2.1	2a/248		
Ethanol	None		4101	2.5	2c/423		
n-Propanol							
i-Propanol	None		6386	1.5	2b/96		
n-Butanol	70	114	8152	2.5	2b/193		
i-Butanol	9	108	8343				
s-Butanol							
n-Amyl alc.				30.2	2f/380		
i-Amyl alc.	None		9836				
Cyclohexanol							
1-Octanol							
Ethanediol						8.65	V2/430
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME	75	114	6575				
EEE	None		8433				
EGBE							
Chlorinated							
MDC							
Chloroform	None		1492	0.5	3+4/343		
Carbon tet.				1.1	1x/3/1233		
1,2-EDC				0.8	3b/519		
1,1,1-TCA				0.9	1x/3/1233		
TCE				1.1	3b/517		
Perk.	52	114	2209				
MCB	None			1.0	3b/543		

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5382	1.2	1x/1/273	0.12	V2/485
MEK				1.1	3+4/300		
MIBK	–		–	–	–	–	–
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				1.2	3b/523		
THF							
Esters							
Me acetate							
Et acetate				1.9	3b/527		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2	None		1272				
Acetic acid	None		3175	1.8	3+4/345	0.32	V2/285
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	40	115	8849	1.0	3b/531		
2-Nitropropane							
Acetonitrile						0.08	V2/183
Furfuraldehyde				1.4	3a/126	0.03	V3/193
Phenol						<0.01	V3/295
Water	76	88	537	10.6	1b/337		

Cyclohexanone

Alternative names
Cyclohexyl ketone, sextone

Reference codes			
CAS number	108 94 1	Hazchem code	3Y
UN number	1915	EPA code	U057
Physical properties			
Molecular weight	98	Cubic expansion coeff (per °C × 10^3)	0.94
Empirical formula	$C_6H_{10}O_1$	Surface tension (@20°C dyn/cm)	34.5
Boiling point (°C)	156	Absolute viscosity (@25°C cP)	2.2
Freezing point (°C)	–32	Refractive index (25°C)	1.448
Specific gravity (20/4)	0.948		
Fire hazards			
Flash point (closed cup °C)	43	Lower explosive limit (ppm)	11000
Autoignition temperature (°C)	420	Upper explosive limit (ppm)	94000
Electrical conductivity	5E–18		
Health hazards			
IDLH (ppm)	5000	Vapour concentration @21°C ppm	3963
OES-TWA	25	Vapour density (relative to air)	3.40
OES-STEL	100	Vapour pressure @21°C mmHg	3.1
Odour threshold (ppm)	1	POCP	

Aqueous effluent	
Solubility in water (25°C %w/w)	2.3
Solubility of water in (25°C %w/w)	8.0
Log_{10} activated carbon partition	3.0
Log_{10} partition in octanol/water (w/w)	+0.81
Biological oxygen demand w/w (days)	1.23
Theoretical oxygen demand w/w	2.61

Vapour pressure equation constants (Log_{10}, mmHg)		
Antoine equation	A	7.47050
	B	1832.200
	C	244.200
Cox chart	A	7.32768
	B	1716.5

Solvent properties			
Solubility parameter	9.9	Kauri butanol value	
Dipole (D)	3.1	Evaporation time (ether = 1)	41
Dielectric constant (20°C)	18.2	Evaporation time (BuAc = 1)	0.25
Polarity (water 100)	28		

Thermal information	
Latent heat (cal/mol)	9016
Nett heat of combustion (kcal/gmol)	788
Specific heat (cal/mol/°C)	48
Critical pressure (MN/m^2)	3.8
Critical temperature (K)	629
Latent heat of fusion (cal/mol)	
Van der Waals' volume	4.14
Van der Waals' surface area	3.34
Molar volume	104.2

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				3.7	1x/1/257		
n-Hexane				4.1	1x/1/258		
n-Heptane				4.4	3b/509		
n-Octane				4.9	1x/3/1210		
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane				1.6	3b/505		
Benzene				0.9	3b/503		
Toluene	None			1.0	3+4/339		
Ethylbenzene							
Xylenes	None		11367	1.5	3b/511		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol							
Ethanol				2.1	1x/3/1210		
n-Propanol							
i-Propanol							
n-Butanol							
i-Butanol							
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol	None		11357				
1-Octanol							
Ethanediol						3.4	V2/428
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE						0.03	P3981
Chlorinated							
MDC				0.4	1x/1/256		
Chloroform				0.3	1x/1/256		
Carbon tet.				1.2	3b/495		
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB	None		10512				

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				1.3	1x/1/256		
MEK				1.0	1x/3/1210		
MIBK							
Cyclohexanone	–		–	–	–	–	–
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE				2.5	3b/506		
Dibutyl ether							
MTBE							
1,4-Dioxane				1.0	1x/3/1210		
THF							
Esters							
Me acetate							
Et acetate				1.3	1x/1/256		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF				1.8	3b/500		
DMAc							
DMSO							
Sulfolane							
CS_2				1.9	1x/1/356		
Acetic acid							
Aniline	None		11144				
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile				1.4	1x/1/256		
Furfuraldehyde	None		8762				
Phenol	28	185	10889	0.1	2b/368		
Water	43	96	506	5.93	1/511		

n-Methyl-2-pyrrolidone

Alternative names
M-pyrol, NMP, 1-methyl pyrrolidone

Reference codes

CAS number	872 50 4	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	99	Cubic expansion coeff (per °C × 10^3)	0.9
Empirical formula	$C_5H_9N_1O_1$	Surface tension (@20°C dyn/cm)	40.7
Boiling point (°C)	202	Absolute viscosity (@25°C cP)	1.8
Freezing point (°C)	–24	Refractive index (25°C)	1.468
Specific gravity (20/4)	1.03		

Fire hazards

Flash point (closed cup °C)	95	Lower explosive limit (ppm)	21800
Autoignition temperature (°C)	287	Upper explosive limit (ppm)	122400
Electrical conductivity	2E–8		

Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	395
OES-TWA	100	Vapour density (relative to air)	3.44
OES-STEL		Vapour pressure @21°C mmHg	0.3
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		
Log_{10} partition in octanol/water (w/w)		
Biological oxygen demand w/w (days)		1.1 (5)
Theoretical oxygen demand w/w		2.18

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

Antoine equation	A	8.27890
	B	2570.30
	C	273.150
Cox chart	A	
	B	

Solvent properties

Solubility parameter	11.0	Kauri butanol value	
Dipole (D)	4.1	Evaporation time (ether = 1)	
Dielectric constant (20°C)	32.2	Evaporation time (BuAc = 1)	0.04
Polarity (water 100)	36		

Thermal information

Latent heat (cal/mol)	12600
Nett heat of combustion (kcal/gmol)	667
Specific heat (cal/mol/°C)	40
Critical pressure (MN/m^2)	
Critical temperature (K)	722
Latent heat of fusion (cal/mol)	6207
Van der Waals' volume	3.98
Van der Waals' surface area	3.20
Molar volume	96.1

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				10.2	1x/1/171		
n-Hexane				11.3	1x/1/174		
n-Heptane				10.5	1x/1/176		
n-Octane				12.1	1x/1/176		
n-Nonane				13.9	1x/1/177		
n-Decane				15.9	1x/1/177		
2,2,4-TMP				14.4	1x/1/177		
Cyclohexane				5.9	1x/1/173		
Benzene				1.2	1x/1/172		
Toluene				1.5	1x/1/175		
Ethylbenzene				1.8	1x/1/176		
Xylenes				1.8	1x/1/1125		
C_9 Aromatics				2.0	3b/463		
Tetralin							
Alcohols							
Methanol				0.5	1x/1/169		
Ethanol				0.6	1x/1/169		
n-Propanol				0.7	1x/3/1118		
i-Propanol				0.75	1x/1/169		
n-Butanol				0.7	1x/3/1119		
i-Butanol				0.7	1x/3/1119		
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol				0.6	2f/411		
1-Octanol							
Ethanediol				0.05	2f/17		
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC				0.4	1x/3/1117		
Chloroform				0.4	1x/3/1117		
Carbon tet.				2.3	1x/3/1117		
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB							

Ketones

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone				1.3	1x/1/169		
MEK				1.4	1x/1/170		
MIBK							
Cyclohexanone							
NMP	–		–	–	–	–	–
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				1.2	1x/3/1119		
THF							
Esters							
Me acetate				1.6	1x/1/169		
Et acetate				1.9	1x/3/1119		
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid							
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde							
Phenol							
Water	None		416a	1.15	1a/379		

Acetophenone

Alternative names
Acetylbenzene, methyl phenyl ketone

Reference codes

CAS number	98 86 2	Hazchem code	
UN number		EPA code	

Physical properties

Molecular weight	120	Cubic expansion coeff (per °C × 10^3)	0.84
Empirical formula	$C_8H_8O_1$	Surface tension (@30°C dyn/cm)	12
Boiling point (°C)	202	Absolute viscosity (@25°C cP)	1.74
Freezing point (°C)	+19.6	Refractive index (25°C)	1.532
Specific gravity (20/4)	1.024		

Fire hazards

Flash point (closed cup °C)	82	Lower explosive limit (ppm)	
Autoignition temperature (°C)	570	Upper explosive limit (ppm)	
Electrical conductivity	3E–9		

Health hazards

IDLH (ppm)	1.0	Vapour concentration @21°C ppm	461
OES-TWA		Vapour density (relative to air)	4.17
OES-STEL		Vapour pressure @21°C mmHg	0.35
Odour threshold (ppm)	10	POCP	

Aqueous effluent

Solubility in water (25°C %w/w)	0.55
Solubility of water in (25°C %w/w)	1.70
Log_{10} activated carbon partition	3.84
Log_{10} partition in octanol/water (w/w)	
Biological oxygen demand w/w (days)	
Theoretical oxygen demand w/w	2.53

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

Antoine equation	A	7.2273
	B	1774.6
	C	206.3
Cox chart	A	
	B	

Solvent properties

Solubility parameter		Kauri butanol value	
Dipole (D)	2.9	Evaporation time (ether = 1)	
Dielectric constant (20°C)	17.4	Evaporation time (BuAc = 1)	0.03
Polarity (water 100)	30.6		

Thermal information

Latent heat (cal/mol)	10032
Nett heat of combustion (kcal/gmol)	949
Specific heat (cal/mol/°C)	54
Critical pressure (MN/m^2)	3.8
Critical temperature (K)	428
Latent heat of fusion (cal/mol)	
Van der Waals' volume	4.69
Van der Waals' surface area	3.61
Molar volume	117.4

Solute	Azeotrope X% w/w	°C	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				5.4	1x/1/363		
n-Hexane				6.4	1x/1/363		
n-Heptane				6.0	1x/1/363		
n-Octane				7.6	1x/3/1345		
n-Nonane				7.3	1x/1/364		
n-Decane							
2,2,4-TMP							
Cyclohexane				4.7	1x/1/363		
Benzene				1.6	1x/1/363		
Toluene				1.3	1x/3/1345		
Ethylbenzene				1.7	1x/1/363		
Xylenes				1.8	1x/1/364		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol				3.5	1x/1/362		
Ethanol				3.3	1x/3/1345		
n-Propanol							
i-Propanol							
n-Butanol							
i-Butanol							
s-Butanol	None			1.1	2b/251		
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol	13	195	13909				
Ethanediol	48	186	4316				
DEG	None		8538				
1,2-Propanediol		184	6664				
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC				0.6	1x/1/362		
Chloroform				0.6	1x/1/362		
Carbon tet.				1.7	1x/1/362		
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB							

Ketones

Solute	Azeotrope X% w/w	°C)	Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone							
MEK				1.00	1x/3/1345		
MIBK							
Cyclohexanone							
NMP							
Acetophenone	–		–	–	–	–	–
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane				0.9	1x/3/1345		
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2				2.1	1x/1/362		
Acetic acid							
Aniline							
Nitrobenzene	None		10733				
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile				1.7	1x/1/362		
Furfuraldehyde						0.02	V3/205
Phenol				0.5	2f/402		
Water	18	98	671	6.44	1a/460		