Section 7

Esters

Methyl acetate

Alternative names
Acetic acid, methyl ester

Reference codes			
CAS number	79 20 9	Hazchem code	2SE
UN number	1231	EPA code	
Physical properties			
Molecular weight	74	Cubic expansion coeff (per °C × 10^3)	1.4
Empirical formula	$C_3H_6O_2$	Surface tension (@20°C dyn/cm)	24
Boiling point (°C)	57	Absolute viscosity (@25°C cP)	0.37
Freezing point (°C)	–98	Refractive index (25°C)	1.360
Specific gravity (20/4)	0.927		
Fire hazards			
Flash point (closed cup °C)	–10	Lower explosive limit (ppm)	31000
Autoignition temperature (°C)	500	Upper explosive limit (ppm)	160000
Electrical conductivity	3.4E–6		
Health hazards			
IDLH (ppm)	10000	Vapour concentration @21°C ppm	290000
OES-TWA	200	Vapour density (relative to air)	2.57
OES-STEL	250	Vapour pressure @21°C mmHg	171
Odour threshold (ppm)	200	POCP	2.5
Aqueous effluent			
Solubility in water (25°C %w/w)		24.5	
Solubility of water in (25°C %w/w)		8.2	
Log_{10} activated carbon partition		1.85	
Log_{10} partition in octanol/water (w/w)		+0.18	
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w		1.51	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.06524	
	B	1157.63	
	C	219.726	
Cox chart	A	7.25014	
	B	1254.0	
Solvent properties			
Solubility parameter	9.6	Kauri butanol value	
Dipole (D)	1.7	Evaporation time (ether = 1)	2.1
Dielectric constant (20°C)	6.7	Evaporation time (BuAc = 1)	9.5
Polarity (water 100)	29		
Thermal information			
Latent heat (cal/mol)	7178		
Nett heat of combustion (kcal/gmol)	348		
Specific heat (cal/mol/°C)	37		
Critical pressure (MN/m^2)	4.6		
Critical temperature (K)	507		
Latent heat of fusion (cal/mol)			
Van der Waals' volume	2.80		
Van der Waals' surface area	2.58		
Molar volume	79.8		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane	22	34	5536				
n-Hexane	63	52	5554				
n-Heptane	96	57	5558	5.5	1x/3/994		
n-Octane							
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	80	55	5541	3.6	5/393		
Benzene	0.3	57	5537	1.4	5/375		
Toluene							
Ethylbenzene							
Xylenes							
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	81	54	1967	2.7	2a/92		
Ethanol	97	57	3969	1.9	2a/335		
n-Propanol	None			2.8	2a/530		
i-Propanol	None		5516	2.2	2b/50		
n-Butanol				2.3	2f/137		
i-Butanol							
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol						3.81	V2/416
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC	None		1557	0.6	5/347		
Chloroform	23	65	1448	0.6	5/341		
Carbon tet.	None		1110	1.7	5/339		
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB				1.2	5/374		

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Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	50	55	5310	1.3	3+4/159	0.37	V2/463
MEK	None		5519	1.0	3+4/271		
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether	None		5527				
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate	–		–	–	–	–	–
Et acetate	None		5521a	0.8	5/357		
i-Propyl acetate							
n-Butyl acetate	None			1.2	5/397		
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2	30	40	1198	2.7	5/349		
Acetic acid	None		3101a	1.1	5/82	0.41	V4/183
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile	None		2763	1.4	5/354		
Furfuraldehyde							
Phenol							
Water	97	56	276	8.5	1/264		

Ethyl acetate

Alternative names
ETAC, acetic ester, EtOAc, ethyl ethanoate, acetic acid, ethyl ester

Reference codes			
CAS number	141 78 6	Hazchem code	3YE
UN number	1173	EPA code	U112
Physical properties			
Molecular weight	88	Cubic expansion coeff (per °C × 10^3)	1.39
Empirical formula	$C_4H_8O_2$	Surface tension (@20°C dyn/cm)	24
Boiling point (°C)	77	Absolute viscosity (@25°C cP)	0.46
Freezing point (°C)	–84	Refractive index (25°C)	1.370
Specific gravity (20/4)	0.895		
Fire hazards			
Flash point (closed cup °C)	–4	Lower explosive limit (ppm)	22000
Autoignition temperature (°C)	484	Upper explosive limit (ppm)	115000
Electrical conductivity	1.0E–9		
Health hazards			
IDLH (ppm)	10000	Vapour concentration @21°C ppm	114000
OES-TWA	400	Vapour density (relative to air)	3.04
OES-STEL		Vapour pressure @21°C mmHg	78
Odour threshold (ppm)	50	POCP	21.8
Aqueous effluent			
Solubility in water (25°C %w/w)		7.7	
Solubility of water in (25°C %w/w)		3.3	
Log_{10} activated carbon partition		2.31	
Log_{10} partition in octanol/water (w/w)		+0.73	
Biological oxygen demand w/w (days)		1.2	
Theoretical oxygen demand w/w		1.82	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.10179	
	B	1244.95	
	C	217.881	
Cox chart	A	7.30648	
	B	1358.7	
Solvent properties			
Solubility parameter	9.1	Kauri butanol value	
Dipole (D)	1.7	Evaporation time (ether = 1)	3.0
Dielectric constant (20°C)	6.02	Evaporation time (BuAc = 1)	4.2
Polarity (water 100)	23		
Thermal information			
Latent heat (cal/mol)	7744		
Nett heat of combustion (kcal/gmol)	493		
Specific heat (cal/mol/°C)	40		
Critical pressure (MN/m^2)	3.84		
Critical temperature (K)	523		
Latent heat of fusion (cal/mol)	2494		
Van der Waals' volume	3.48		
Van der Waals' surface area	3.12		
Molar volume	98.5		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane				3.1	1x/1/105		
n-Hexane	38	65	7588	2.4	5/514		
n-Heptane				2.9	1x/3/1051		
n-Octane				3.1	1x/3/1051		
n-Nonane							
n-Decane							
2,2,4-TMP				1.5	1x/3/1051		
Cyclohexane	54	72	7583	2.3	5/506		
Benzene	None		7580	3.1	5/502		
Toluene	None		7591	1.2	5/516		
Ethylbenzene				1.8	5/540		
Xylenes	None		7594	1.6	5/541		
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	56	62	1999	2.7	1x/1/103	1.08	V2/93
Ethanol	69	72	4012	2.2	2a/351	0.41	CEH
n-Propanol	None		6448	1.9	2a/536	0.19	V2/549
i-Propanol	75	76	6338	1.6	2b/59	0.17	CEH
n-Butanol	None		7567	2.3	2b/148	0.03	V3/50
i-Butanol	None		7570			0.04	V3/54
s-Butanol	None		7568			0.07	V3/52
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol	None			3.5	2d/511		
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME				2.0	2b/126		
EEE	None		7571	2.2	2f/335		
EGBE	None		7590				
Chlorinated							
MDC				0.5	1x/1/103		
Chloroform	72	78	1466	0.5	1x/1/103		
Carbon tet.	43	75	1125	1.3	1x/1/103		
1,2-EDC	None		2980	0.8	1x/1/103		
1,1,1-TCA							
TCE	None		2302	0.9	5/454		
Perk.							
MCB	None		7578	1.4	5/492		

Esters

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5334	1.2	3+4/176	0.14	CEH
MEK	82	77	7345	2.0	3+4/278		
MIBK				0.6	3b/527		
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether				1.0	3+4/513		
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane	None		7514	1.1	3+4/455		
THF				1.1	1x/1/104		
Esters							
Me acetate	None		5521a	1.1	5/357		
Et acetate	–		–	–	–	–	–
i-Propyl acetate	None			1.0	5/487		
n-Butyl acetate	None		7585				
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc						1.85	V3/48
DMSO				3.9	5/461		
Sulfolane							
CS_2	3	46	1220	2.7	1x/1/103		
Acetic acid	None		3120	7.0	5/104	0.29	V4/184
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane	None		6274				
Acetonitrile	77	75	2770	1.6	1x/1/103	0.17	V2/175
Furfuraldehyde	None		7574	1.7	3a/123	0.03	V2/57
Phenol						<0.01	V4/241
Water	91.5	70	352	9.7	1/393		

Isopropyl acetate

Alternative names
Sec propyl acetate, 2-propyl acetate, acetic acid, isopropyl ester

Reference codes			
CAS number	108 21 4	Hazchem code	3YE
UN number	1220	EPA code	
Physical properties			
Molecular weight	102	Cubic expansion coeff (per °C × 10^3)	1.31
Empirical formula	$C_5H_{10}O_2$	Surface tension (@20°C dyn/cm)	22.1
Boiling point (°C)	89	Absolute viscosity (@25°C cP)	0.46
Freezing point (°C)	–69	Refractive index (25°C)	1.375
Specific gravity (20/4)	0.874		
Fire hazards			
Flash point (closed cup °C)	3	Lower explosive limit (ppm)	18000
Autoignition temperature (°C)	460	Upper explosive limit (ppm)	80000
Electrical conductivity	5.7E–7		
Health hazards			
IDLH (ppm)	16000	Vapour concentration @21°C ppm	66000
OES-TWA	250	Vapour density (relative to air)	3.5
OES-STEL	200	Vapour pressure @21°C mmHg	47
Odour threshold (ppm)	30	POCP	21.5
Aqueous effluent			
Solubility in water (25°C %w/w)		2.9	
Solubility of water in (25°C %w/w)		3.2	
Log_{10} activated carbon partition		2.63	
Log_{10} partition in octanol/water (w/w)			
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w		2.04	
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	7.3340	
	B	1436.53	
	C	233.7	
Cox chart	A	7.34068	
	B	1422.7	
Solvent properties			
Solubility parameter	8.5	Kauri butanol value	
Dipole (D)	2.7	Evaporation time (ether = 1)	
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	
Polarity (water 100)			
Thermal information			
Latent heat (cal/mol)	8262		
Nett heat of combustion (kcal/gmol)	534		
Specific heat (cal/mol/°C)	50		
Critical pressure (MN/m^2)	3.65		
Critical temperature (K)	538		
Latent heat of fusion (cal/mol)			
Van der Waals' volume	4.15		
Van der Waals' surface area	3.65		
Molar volume	117.8		

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane	9	69	9297				
n-Heptane	67	88	9302				
n-Octane							
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	25	79	9296				
Benzene	None		9294				
Toluene	None		9300				
Ethylbenzene							
Xylenes							
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	20	65	2046				
Ethanol	48	77	4054	1.9	2a/391		
n-Propanol							
i-Propanol	48	80	6363	1.7	2f/59		
n-Butanol	None		8121				
i-Butanol							
s-Butanol							
n-Amyl alc.							
i-Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
Glycol ethers							
PGME							
EGME							
EEE							
EGBE							
Chlorinated							
MDC							
Chloroform							
Carbon tet.	None		1145				
1,2-EDC	None		2992				
1,1,1-TCA							
TCE	None		2317				
Perk.							
MCB							

Esters

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Ketones							
Acetone	None		5365				
MEK	None		7366				
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane	None		7527				
THF							
Esters							
Me acetate							
Et acetate	None			1.0	5/487		
i-Propyl acetate	–		–	–	–	–	–
n-Butyl acetate							
Cellosolve acetate							
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2	None		1251				
Acetic acid	None		3147	1.4	5/123	0.36	V2/236
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile	20	80	2788				
Furfuraldehyde							
Phenol						<0.01	V4/264
Water	90	77	439				

n-Butyl acetate

Alternative names
BuAc, *n*-butyl ethanoate, BuOAc, acetic acid, butyl ester

Reference codes			
CAS number	123 86 4	Hazchem code	3YE
UN number	1123	EPA code	
Physical properties			
Molecular weight	116	Cubic expansion coeff (per °C × 10^3)	1.16
Empirical formula	$C_6H_{12}O_2$	Surface tension (@20°C dyn/cm)	25.1
Boiling point (°C)	126	Absolute viscosity (@25°C cP)	0.73
Freezing point (°C)	–73	Refractive index (25°C)	1.392
Specific gravity (20/4)	0.876		
Fire hazards			
Flash point (closed cup °C)	22	Lower explosive limit (ppm)	17000
Autoignition temperature (°C)	407	Upper explosive limit (ppm)	150000
Electrical conductivity	1.6E–8		
Health hazards			
IDLH (ppm)	10000	Vapour concentration @21°C ppm	14200
OES-TWA	150	Vapour density (relative to air)	4.03
OES-STEL	200	Vapour pressure @21°C mmHg	10.6
Odour threshold (ppm)	15	POCP	32.3

Aqueous effluent	
Solubility in water (25°C %w/w)	0.7
Solubility of water in (25°C %w/w)	1.3
Log_{10} activated carbon partition	3.04
Log_{10} partition in octanol/water (w/w)	+1.7
Biological oxygen demand w/w (days)	1.15
Theoretical oxygen demand w/w	2.21

Vapour pressure equation constants (Log_{10}, mmHg)		
Antoine equation	A	7.02845
	B	1368.50
	C	204.00
Cox chart	A	7.44951
	B	1626.5

Solvent properties			
Solubility parameter	8.6	Kauri butanol value	
Dipole (D)	1.8	Evaporation time (ether = 1)	11.8
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	1.0
Polarity (water 100)	24.1		

Thermal information	
Latent heat (cal/mol)	8584
Nett heat of combustion (kcal/gmol)	784
Specific heat (cal/mol/°C)	58
Critical pressure (MN/m^2)	3.05
Critical temperature (K)	579
Latent heat of fusion (cal/mol)	
Van der Waals' volume	4.83
Van der Waals' surface area	4.20
Molar volume	132.5

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Partition coefficient	Reference
Hydrocarbons							
n-Pentane							
n-Hexane							
n-Heptane	None		11826a	1.8	5/591		
n-Octane	52	119	11832				
n-Nonane							
n-Decane							
2,2,4-TMP							
Cyclohexane	None		11687	1.5	5/585		
Benzene	None		10859	0.9	5/583		
Toluene				1.0	5/586		
Ethylbenzene	None		11828				
Xylenes	None		11830				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol	None			5.8	2c/213	1.12	V2/131
Ethanol	None			2.1	2c/426	0.61	V2/363
n-Propanol	60	94		1.2	2e/484	0.11	V2/574
i-Propanol	None			1.8	2d/75		
n-Butanol	37	116	8153	1.4	2b/197	0.03	V4/253
i-Butanol	None		8345				
s-Butanol	None		8237				
n-Amyl alc.	None		9754				
i-Amyl alc.	82	126	9837				
Cyclohexanol	None			1.5	2f/417		
1-Octanol							
Ethanediol	None		4258	6.9	2d/15		
DEG							
1,2-Propanediol	None		6655a				
Glycol ethers							
PGME	None		9968				
EGME	52	119	6576	2.3	2d/122		
EEE	87	126	8434	1.8	2b/294		
EGBE	None		11823				
Chlorinated							
MDC							
Chloroform	None		1493	0.7	5/574		
Carbon tet.	None		1161	1.2	5/573		
1,2-EDC							
1,1,1-TCA							
TCE				0.7	5/575		
Perk.	21	120	2210				
MCB	None		10516				

Esters

Solute	Azeotrope X% w/w	Azeotrope °C	Azeotrope Reference	Solute γ^{∞}	Reference	Part coefficient	Reference
Ketones							
Acetone	None		5383	1.4	3b/197	0.14	CEH
MEK							
MIBK							
Cyclohexanone							
NMP							
Acetophenone							
Ethers							
Diethyl ether							
DIPE							
Dibutyl ether	95	126	11833				
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate	None			1.2	5/397		
Et acetate	None		7585				
i-Propyl acetate							
n-Butyl acetate	–		–	–	–	–	–
Cellosolve acetate	None		11821				
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid	None		3177	2.1	5/147	0.23	V4/185
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	None		8850				
2-Nitropropane							
Acetonitrile				2.3	5/577	0.07	V2/184
Furfuraldehyde				1.8	3+4/46	0.02	V3/194
Phenol	Azeo		10896	0.5	2b/373	<0.01	V3/297
Water	71	90	542	6.7	1/516		

Cellosolve acetate

Alternative names
Ethylene glycol monoethyl acetate, 2-ethoxy ethyl acetate

Reference codes			
CAS number	111 15 9	Hazchem code	
UN number	1172	EPA code	
Physical properties			
Molecular weight	132	Cubic expansion coeff (per °C × 10^3)	1.12
Empirical formula	$C_6H_{12}O_3$	Surface tension (@20°C dyn/cm)	28.2
Boiling point (°C)	156	Absolute viscosity (@25°C cP)	
Freezing point (°C)	–62	Refractive index (20°C)	
Specific gravity (20/4)	0.973		
Fire hazards			
Flash point (closed cup °C)	52	Lower explosive limit (ppm)	17000
Autoignition temperature (°C)	345	Upper explosive limit (ppm)	82000
Electrical conductivity			
Health hazards			
IDLH (ppm)	2500	Vapour concentration @21°C ppm	2108
OES-TWA	5	Vapour density (relative to air)	4.6
OES-STEL		Vapour pressure @21°C mmHg	1.5
Odour threshold (ppm)	0.1	POCP	60
Aqueous effluent			
Solubility in water (25°C %w/w)	22.9		
Solubility of water in (25°C %w/w)	6.5		
Log_{10} activated carbon partition			
Log_{10} partition in octanol/water (w/w)			
Biological oxygen demand w/w (days)			
Theoretical oxygen demand w/w	1.82		
Vapour pressure equation constants (Log_{10}, mmHg)			
Antoine equation	A	6.8246	
	B	1291.3	
	C	170.97	
Cox chart	A	7.542	
	B	1799.3	
Solvent properties			
Solubility parameter	8.6	Kauri butanol value	
Dipole (D)	1.8	Evaporation time (ether = 1)	57
Dielectric constant (20°C)		Evaporation time (BuAc = 1)	0.2
Polarity (water 100)			
Thermal information			
Latent heat (cal/mol)	9768		
Nett heat of combustion (kcal/gmol)	754		
Specific heat (cal/mol/°C)	63.9		
Critical pressure (MN/m^2)	3.0		
Critical temperature (K)	607		
Latent heat of fusion (cal/mol)			
Van der Waals' volume			
Van der Waals' surface area			
Molar volume	135.7		

Solute	Azeotrope X% w/w	°C	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							
Toluene	None		11913				
Ethylbenzene	None		12007				
Xylenes	None		12009				
C_9 Aromatics							
Tetralin							
Alcohols							
Methanol							
Ethanol							
n-Propanol							
i-Propanol							
n-Butanol	None		8160				
i-Butanol	None		8352				
s-Butanol							
n-Amyl alc.							
i-Amyl alc.	None		9842				
Cyclohexanol							
1-Octanol							
Ethanediol	None		4261				
DEG							
1,2-Propanediol	None		6665				
Glycol ethers							
PGME	13	151	9969				
EGME	None		6583				
EEE	None		8440				
EGBE	None		11989				
Chlorinated							
MDC							
Chloroform							
Carbon tet.							
1,2-EDC							
1,1,1-TCA							
TCE							
Perk.							
MCB							

Esters

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	88	142	12021				
MTBE							
1,4-Dioxane							
THF							
Esters							
Me acetate							
Et acetate							
i-Propyl acetate							
n-Butyl acetate	None		11821				
Cellosolve acetate	–		–	–	–	–	–
Miscellaneous							
DMF							
DMAc							
DMSO							
Sulfolane							
CS_2							
Acetic acid							
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile							
Furfuraldehyde	None		8766				
Phenol	28	185	10898				
Water	50	97	559				