

# **Chlorinated solvents**

# Methylene chloride

## Alternative names

Dichloromethane, MDC, methylene dichloride, **not** methyl chloride

## Reference codes

CAS number	75 09 2	Hazchem code	2Z
UN number	1593	EPA code	U080

## Physical properties

Molecular weight	85	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.37
Empirical formula	C <sub>1</sub> H <sub>2</sub> Cl <sub>2</sub>	Surface tension (@20°C dyn/cm)	28.1
Boiling point (°C)	40	Absolute viscosity (@25°C cP)	0.44
Freezing point (°C)	-95	Refractive index (25°C)	1.4211
Specific gravity (20/4)	1.326		

## Fire hazards

Flash point (closed cup °C)	None	Lower explosive limit (ppm)	130000
Autoignition temperature (°C)	605	Upper explosive limit (ppm)	220000
Electrical conductivity	4.3E-11		

## Health hazards

IDLH (ppm)	5000	Vapour concentration @21°C ppm	495000
OES-TWA	50	Vapour density (relative to air)	2.95
OES-STEL	300	Vapour pressure @21°C mmHg	376
Odour threshold (ppm)	250	POCP	0.9

## Aqueous effluent

Solubility in water (25°C %w/w)	1.30		
Solubility of water in (25°C %w/w)	0.20		
Log <sub>10</sub> activated carbon partition	2.9		
Log <sub>10</sub> partition in octanol/water (w/w)	+1.25		
Biological oxygen demand w/w (days)			0 (5)
Theoretical oxygen demand w/w	0.56		

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	7.0803
	B	1138.91
	C	231.45
Cox chart	A	6.91821
	B	1090.1

## Solvent properties

Solubility parameter	9.7	Kauri butanol value	136
Dipole (D)	1.8	Evaporation time (ether = 1)	1.8
Dielectric constant (20°C)	9.1	Evaporation time (BuAc = 1)	25.0
Polarity (water 100)	30.9		

## Thermal information

Latent heat (cal/mol)	6715
Nett heat of combustion (kcal/gmol)	122
Specific heat (cal/mol/°C)	24
Critical pressure (MN/m <sup>2</sup> )	6.08
Critical temperature (K)	510
Latent heat of fusion (cal/mol)	1436
Van der Waals' volume	2.26
Van der Waals' surface area	1.99
Molar volume	64.50

Solute	Azeotrope		Reference	Solute $\gamma^m$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane	49	36	1571	2.9	6a/100		
<i>n</i> -Hexane	None		1575				
<i>n</i> -Heptane							
<i>n</i> -Octane				4.1	1x/3/923		
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP							
Cyclohexane							
Benzene							
Toluene				1.0	1x/3/923		
Ethylbenzene							
Xylenes							
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	93	38	1544	7.9	2e/24	9.28	V4/118
Ethanol	95	40	1551	43.7	2c/283		
<i>n</i> -Propanol				4.1	2e/416		
<i>i</i> -Propanol	None		1561	4.1	2f/36		
<i>n</i> -Butanol							
<i>i</i> -Butanol							
<i>s</i> -Butanol							
<i>n</i> -Amyl alc.							
<i>i</i> -Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME							
EEE							
EGBE							
<i>Chlorinated</i>							
MDC	-		-	-	-	-	-
Chloroform	None		1426	0.7	8/202		
Carbon tet.				0.9	8/62		
1,2-EDC				1.0	8/263		
1,1,1-TCA				1.2	1x/3/923		
TCE				1.5	1x/3/923		
Perk.				0.9	8/256		
MCB							

Chlorinated solvents

Solute	Azeotrope		Solute $\gamma^{\infty}$	Reference	Partition coefficient	Reference
	X% w/w	°C				
<i>Ketones</i>						
Acetone	None		1553	1.1	3b/27	
MEK	None		1564	0.4	3+4/261	
MIBK						
Cyclohexanone						
NMP						
Acetophenone						
<i>Ethers</i>						
Diethyl ether	70	41	1566	0.7	3+4/492	
DIPE						
Dibutyl ether						
MTBE						
1,4-Dioxane				0.4	1x/3/923	
THF					0.09	
<i>Esters</i>						
Me acetate	None		1557	0.5	5/347	
Et acetate				0.4	5/449	
<i>i</i> -Propyl acetate						
<i>n</i> -Butyl acetate						
Cellosolve acetate						
<i>Miscellaneous</i>						
DMF				0.8	8/265	0.39
DMAc						V4/120
DMSO				0.45	8/264	
Sulfolane				0.8	8/266	
CS <sub>2</sub>	65	36	1170			
Acetic acid				4.2	5/64	3.24
Aniline						V2/36
Nitrobenzene						
Morpholine						
Pyridine				0.6	8/267	
2-Nitropropane						
Acetonitrile	None		1546	1.2	8/258	
Furfuraldehyde				1.2	3a/115	
Phenol						
Water	99	38	208	1324.0	1/1	

# Chloroform

## Alternative names

Trichloromethane

## Reference codes

CAS number	67 66 3	Hazchem code	2Z
UN number	1888	EPA code	U044

## Physical properties

Molecular weight	119	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.29
Empirical formula	C <sub>1</sub> H <sub>1</sub> Cl <sub>3</sub>	Surface tension (@20°C dyn/cm)	27.16
Boiling point (°C)	61	Absolute viscosity (@25°C cP)	0.57
Freezing point (°C)	-23	Refractive index (25°C)	1.444
Specific gravity (20/4)	1.480		

## Fire hazards

Flash point (closed cup °C)	None	Lower explosive limit (ppm)	None
Autoignition temperature (°C)	None	Upper explosive limit (ppm)	None
Electrical conductivity	<1.0E-10		

## Health hazards

IDLH (ppm)	1000	Vapour concentration @21°C ppm	286000
OES-TWA	2	Vapour density (relative to air)	4.13
OES-STEL		Vapour pressure @21°C mmHg	169
Odour threshold (ppm)	300	POCP	1.0

## Aqueous effluent

Solubility in water (25°C %w/w)	0.82
Solubility of water in (25°C %w/w)	0.072
Log <sub>10</sub> activated carbon partition	3.6
Log <sub>10</sub> partition in octanol/water (w/w)	+1.97
Biological oxygen demand w/w (days)	0.02 (5)
Theoretical oxygen demand w/w	1.35

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	6.95465
	B	1170.966
	C	226.232
Cox chart	A	6.97909
	B	1192.6

## Solvent properties

Solubility parameter	9.3	Kauri butanol value	
Dipole (D)	1.1	Evaporation time (ether = 1)	1.9
Dielectric constant (20°C)	4.8	Evaporation time (BuAc = 1)	
Polarity (water 100)	25.9		

## Thermal information

Latent heat (cal/mol)	70.21
Nett heat of combustion (kcal/gmol)	91
Specific heat (cal/mol/°C)	27
Critical pressure (MN/m <sup>2</sup> )	2.38
Critical temperature (K)	536
Latent heat of fusion (cal/mol)	2097
Van der Waals' volume	2.87
Van der Waals' surface area	2.41
Molar volume	80.41

Solute	Azeotrope		Reference	Solute $\gamma^{\infty}$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane	None		1482	2.1	1x/3/992		
<i>n</i> -Hexane	83	60	1495	1.9	6a/426		
<i>n</i> -Heptane	None		1500	1.4	6b/77		
<i>n</i> -Octane				2.1	1x/3/922		
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP							
Cyclohexane	None		1490				
Benzene	None		1486	0.86	1x/1/4		
Toluene	None		1498	0.75	7/352		
Ethylbenzene							
Xylenes							
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	87	53	1430	7.4	2a/23	3.5	P160
Ethanol	93	59	1442	4.3	2a/285	1.07	P373
<i>n</i> -Propanol	None		1454			0.24	P640
<i>i</i> -Propanol	96	61	1453	6.6	2d/40	0.34	P651
<i>n</i> -Butanol				2.7	2b/136	0.05	P952
<i>i</i> -Butanol	None		1475			0.07	P964
<i>s</i> -Butanol	None		1472			0.08	P976
<i>n</i> -Amyl alc.							
<i>i</i> -Amyl alc.							
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME							
EEE							
EGBE							
<i>Chlorinated</i>							
MDC	None		1426	0.8	8/202		
Chloroform	-		-	-	-	-	-
Carbon tet.	None		1086	1.1	8/56		
1,2-EDC	None		1435	1.1	1x/3/921		
1,1,1-TCA				1.0	1x/3/921		
TCE				1.1	1x/3/921		
Perk.	None		1431	1.2	8/215		
MCB	None		1484	0.8	8/244		

Chlorinated solvents

Solute	Azeotrope		Reference	Solute $\gamma^{\infty}$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Ketones</i>							
Acetone	78	64	1443	0.5	3+4/90	0.03	P493
MEK	17	80	1460	0.4	3+4/260		
MIBK	None		1492	0.3	3+4/343		
Cyclohexanone							
NMP				0.06	3b/426		
Acetophenone							
<i>Ethers</i>							
Diethyl ether	None		1474	0.4	3+4/486		
DIPE	36	71	1496	0.5	3+4/537		
Dibutyl ether	None		1501a	0.4	3+4/591		
MTBE							
1,4-Dioxane	None		1465	0.3	3+4/441		
THF	66	73	1464	0.25	1x/1/4	0.03	V4/115
<i>Esters</i>							
Me acetate	77	65	1448	0.43	5/341		
Et acetate	28	78	1466	0.23	5/443		
<i>i</i> -Propyl acetate							
<i>n</i> -Butyl acetate	None		1493	0.41	5/574		
Cellosolve acetate							
<i>Miscellaneous</i>							
DMF						0.32	V4/113
DMAc							
DMSO				0.18	8/229		
Sulfolane							
CS <sub>2</sub>	None		1169	1.3	8/213		
Acetic acid	None		1437	4.2	5/62	1.04	V2/18
Aniline						0.007	P1714
Nitrobenzene	None		1485				
Morpholine							
Pyridine	None		1480a	0.35	8/240	0.006	P1102
2-Nitropropane							
Acetonitrile	None		1433	1.2	8/217		
Furfuraldehyde	None		1480	10.7	3+4/36		
Phenol						0.07	P1627
Water	97	56	207				

# Carbon tetrachloride

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## Alternative names

Carbon tet., CTET, tetrachloromethane

## Reference codes

CAS number	56 23 5	Hazchem code	2Z
UN number	1846	EPA code	U211

## Physical properties

Molecular weight	154	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.27
Empirical formula	C <sub>1</sub> Cl <sub>4</sub>	Surface tension (@20°C dyn/cm)	27
Boiling point (°C)	76	Absolute viscosity (@25°C cP)	0.97
Freezing point (°C)	-23	Refractive index (25°C)	1.459
Specific gravity (20/4)	1.58		

## Fire hazards

Flash point (closed cup °C)	None	Lower explosive limit (ppm)	None
Autoignition temperature (°C)	None	Upper explosive limit (ppm)	None
Electrical conductivity	4.0E-18		

## Health hazards

IDLH (ppm)	300	Vapour concentration @21°C ppm	150900
OES-TWA	2	Vapour density (relative to air)	5.34
OES-STEL		Vapour pressure @21°C mmHg	99.6
Odour threshold (ppm)	96	POCP	

## Aqueous effluent

Solubility in water (25°C %w/w)	0.077
Solubility of water in (25°C %w/w)	0.008
Log <sub>10</sub> activated carbon partition	4.3
Log <sub>10</sub> partition in octanol/water (w/w)	+2.64
Biological oxygen demand w/w (days)	0 (5)
Theoretical oxygen demand w/w	0.21

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine Equation	A	6.84083
	B	1210.595
	C	229.664
Cox chart	A	7.02433
	B	1267.9

## Solvent properties

Solubility parameter	8.6	Kauri butanol value	
Dipole (D)	0	Evaporation time (ether = 1)	1.8
Dielectric constant (20°C)	2.24	Evaporation Time (BuAc = 1)	
Polarity (water 100)	5.2		

## Thermal information

Latent heat (cal/mol)	7238
Nett heat of combustion (kcal/gmol)	62
Specific heat (cal/mol/°C)	32
Critical pressure (MN/m <sup>2</sup> )	4.56
Critical temperature (K)	556
Latent heat of fusion (cal/mol)	784
Van der Waals' volume	3.39
Van der Waals' surface area	2.91
Molar volume	97.5



Solute	Azeotrope		Reference	Solute $\gamma^{\circ}$	Reference	Partition coefficient	Reference
	X% w/w	$^{\circ}\text{C}$					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane	None		1162	1.3	6a/403		
<i>n</i> -Hexane	None		1167	1.3	6b/67		
<i>n</i> -Heptane	None		1168a	1.0	6b/234		
<i>n</i> -Octane	None						
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP	None		1168b	1.4	6b/285		
Cyclohexane	None		1159	1.1	6a/142		
Benzene	None		1154	1.1	7/7		
Toluene	None		1166	1.0	7/332		
Ethylbenzene	None		1167a	0.9	7/464		
Xylenes	None		1167c	0.9	7/480		
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	79	56	1090	10.3	2a/1		
Ethanol	84	65	1105	20.5	2a/276	4.76	P382
<i>n</i> -Propanol	92	73	1116	14.5	2a/509		
<i>i</i> -Propanol	82	67	1115	6.7	2b/36	2.45	V2/10
<i>n</i> -Butanol	98	77	1133	9.5	2f/109	0.32	P958
<i>i</i> -Butanol	95	76	1137				
<i>s</i> -Butanol	92	75	1134	5.4	2f/217		
<i>n</i> -Amyl alc.	None		1147a			0.05	P1269
<i>i</i> -Amyl alc.	None		1149				
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME				4.9	2f/99		
EEE							
EGBE							
<i>Chlorinated</i>							
MDC				1.1	8/63		
Chloroform	None		1086	1.0	8/55		
Carbon tet.	-		-	-	-	-	-
1,2-EDC	80	75	1098	1.5	8/96		
1,1,1-TCA	Azeo			1.2	8/82		
TCE	None		1093	0.7	8/80		
Perk.	None		1091	1.0	8/78		
MCB	None		1152	1.4	8/164		

*Chlorinated solvents*

Solute	Azeotrope		Reference	Solute $\gamma^r$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Ketones</i>							
Acetone	12	56	1108	2.3	3+4/80	0.26	P502
MEK	71	74	1121	1.8	3+4/259		
MIBK							
Cyclohexanone				0.9	3b/495		
NMP							
Acetophenone							
<i>Ethers</i>							
Diethyl ether	None		1136				
DIPE	None		1163	1.1	3+4/529		
Dibutyl ether							
MTBE							
1,4-Dioxane	None		1124	1.6	3+4/440		
THF				0.9	3+4/429	0.06	V4/107
<i>Esters</i>							
Me acetate	None		1110	1.6	5/339	0.05	P519
Et acetate	57	75	1125	1.4	5/436		
<i>i</i> -Propyl acetate	None		1145				
<i>n</i> -Butyl acetate	None		1161	0.8	5/573		
Cellosolve acetate							
<i>Miscellaneous</i>							
DMF				5.4	8/117	5.9	V4/106
DMAc							
DMSO				18.5	8/107	3.8	P387
Sulfolane							
CS <sub>2</sub>	None		1085	1.2	8/76		
Acetic acid	98	76	1099	12.2	5/59	6.0	V2/12
Aniline	None			6.0	8/174	0.07	P1720
Nitrobenzene	None		1153	0.7	8/168		
Morpholine							
Pyridine				2.0	8/141		
2-Nitropropane	None		1114	3.2	8/120		
Acetonitrile	83	65	1095	9.6	8/86		
Furfuraldehyde	None		1140	3.8	3+4/35	0.04	
Phenol	None		1155	3.4	2b/355	0.31	P1652
Water	96	66	205				

# 1,2-Dichloroethane

## Alternative names

Ethylene dichloride, EDC

## Reference codes

CAS number	107 06 2	Hazchem code	2YE
UN number	1184	EPA code	U077

## Physical properties

Molecular weight	99	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.16
Empirical formula	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	Surface tension (@20°C dyn/cm)	32.2
Boiling point (°C)	83.5	Absolute viscosity (@25°C cP)	0.9
Freezing point (°C)	-36	Refractive index (25°C)	1.444
Specific gravity (20/4)	1.253		

## Fire hazards

Flash point (closed cup °C)	13	Lower explosive limit (ppm)	62000
Autoignition temperature (°C)	413	Upper explosive limit (ppm)	169000
Electrical conductivity	4E-11		

## Health hazards

IDLH (ppm)	1000	Vapour concentration @21°C ppm	94000
OES-TWA	5	Vapour density (relative to air)	3.4
OES-STEL		Vapour pressure @21°C mmHg	71
Odour threshold (ppm)	400	POCP	

## Aqueous effluent

Solubility in water (25°C %w/w)	0.81
Solubility of water in (25°C %w/w)	0.15
Log <sub>10</sub> activated carbon partition	3.8
Log <sub>10</sub> partition in octanol/water (w/w)	3.6
Biological oxygen demand w/w (days)	0.002 (5)
Theoretical oxygen demand w/w	0.97

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	7.02530
	B	1271.254
	C	222.927
Cox chart	A	7.04532
	B	1303.5

## Solvent properties

Solubility parameter	9.8	Kauri butanol value	
Dipole (D)	1.8	Evaporation time (ether = 1)	2.7
Dielectric constant (20°C)	10.45	Evaporation time (BuAc = 1)	
Polarity (water 100)	32.7		

## Thermal information

Latent heat (cal/mol)	7623
Nett heat of combustion (kcal/gmol)	269
Specific heat (cal/mol/°C)	31
Critical pressure (MN/m <sup>2</sup> )	5.38
Critical temperature (K)	563
Latent heat of fusion (cal/mol)	2091
Van der Waals' volume	2.93
Van der Waals' surface area	2.53
Molar volume	78.87

Solute	Azeotrope		Reference	Solute $\gamma^{\infty}$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane				4.8	1x/1/18		
<i>n</i> -Hexane	None		3003	3.6	1x/1/19		
<i>n</i> -Heptane	76	81	3009	3.4	6c/444		
<i>n</i> -Octane							
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP				3.4	1x/1/19		
Cyclohexane	50	74	3001	3.1	6a/159		
Benzene	20	80	2999	1.1	7/142		
Toluene	None		3006	1.1	7/380		
Ethylbenzene				1.0	7/466		
Xylenes				1.3	7/490		
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	68	61	1930	11.2	2e/44	7.9	V2/83
Ethanol	63	71	2964	4.9	2a/299		
<i>n</i> -Propanol	None		2971	5.1	2a/520		
<i>i</i> -Propanol	57	73	2970	4.9	1x/1/18	1.2	V2/207
<i>n</i> -Butanol	None		2984	3.2	2b/137		
<i>i</i> -Butanol	94	83	2988	4.2	2b/272		
<i>s</i> -Butanol	88	82	2985	2.7	2f/220		
<i>n</i> -Amyl alc.				3.6	2f/375		
<i>i</i> -Amyl alc.	None		2995				
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME							
EEE							
EGBE							
<i>Chlorinated</i>							
MDC				1.0	8/263		
Chloroform	None		1435	1.0	1x/3/957		
Carbon tet.	20	75	1098	1.8	1x/3/957		
1,2-EDC	-		-	-	-	-	-
1,1,1-TCA				1.6	8/363		
TCE	67	82	2281	1.4	8/351		
Perk.				1.7	8/340		
MCB							

Chlorinated solvents

Solute	Azeotrope		Solute $\gamma^{\circ}$	Reference	Partition coefficient	Reference
	X% w/w	$^{\circ}\text{C}$				
<i>Ketones</i>						
Acetone	None		0.8	3+4/144		
MEK	Azeo		0.8	3b/271		
MIBK			0.8	3b/519		
Cyclohexanone						
NMP						
Acetophenone					<0.01	P2746
<i>Ethers</i>						
Diethyl ether	None			2987		
DIPE	None			3004		
Dibutyl ether						
MTBE						
1,4-Dioxane	None		0.9	3+4/447	0.98	V4/180
THF		2979	0.7	1x/3/957		
<i>Esters</i>						
Me acetate						
Et acetate	None		0.8	1x/1/18		
<i>i</i> -Propyl acetate	None			2992		
<i>n</i> -Butyl acetate						
Cellosolve acetate						
<i>Miscellaneous</i>						
DMF						
DMAc						
DMSO						
Sulfolane						
CS <sub>2</sub>			2.6	1x/1/17		
Acetic acid	None		4.4	5/74	1.61	V2/202
Aniline		2961			<0.01	P1721
Nitrobenzene						
Morpholine						
Pyridine			0.9	1x/1/18		
2-Nitropropane						
Acetonitrile	51	79	1.4	8/364		
Furfuraldehyde			1.1	3a/119	0.14	V4/181
Phenol						
Water	91	72		227		

# 1,1,1-Trichloroethane

## Alternative names

Methyl chloroform, TCA, chloroethene, M.C., not 1,1,2-trichloroethane

## Reference codes

CAS number	71 55 6	Hazchem code	2Z
UN number	2831	EPA code	U226

## Physical properties

Molecular weight	133	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.3
Empirical formula	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	Surface tension (@20°C dyn/cm)	30
Boiling point (°C)	74	Absolute viscosity (@25°C cP)	0.65
Freezing point (°C)	-30	Refractive index (25°C)	1.438
Specific gravity (20/4)	1.338		

## Fire hazards

Flash point (closed cup °C)	None	Lower explosive limit (ppm)	65000
Autoignition temperature (°C)	537	Upper explosive limit (ppm)	155000
Electrical conductivity	7.3E-9		

## Health hazards

IDLH (ppm)		Vapour concentration @21°C ppm	154700
OES-TWA	350	Vapour density (relative to air)	4.62
OES-STEL	450	Vapour pressure @21°C mmHg	101.8
Odour threshold (ppm)	300	POCP	0.1

## Aqueous effluent

Solubility in water (25°C %w/w)	0.13
Solubility of water in (25°C %w/w)	0.03
Log <sub>10</sub> activated carbon partition	4.3
Log <sub>10</sub> partition in octanol/water (w/w)	4.0
Biological oxygen demand w/w (days)	
Theoretical oxygen demand w/w	0.48

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	6.90633
	B	1211.31
	C	226.816
Cox chart	A	7.01846
	B	1257.7

## Solvent properties

Solubility parameter	7.7	Kauri butanol value	124
Dipole (D)	1.7	Evaporation time (ether = 1)	2.6
Dielectric constant (20°C)	7.25	Evaporation time (BuAc = 1)	6.0
Polarity (water 100)	17.0		

## Thermal information

Latent heat (cal/mol)	7780
Nett heat of combustion (kcal/gmol)	233
Specific heat (cal/mol/°C)	32
Critical pressure (MN/m <sup>2</sup> )	4.4
Critical temperature (K)	550
Latent heat of fusion (cal/mol)	651.7
Van der Waals' volume	3.54
Van der Waals' surface area	3.03
Molar volume	100.4

Solute	Azeotrope		Reference	Solute $\gamma^*$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane							
<i>n</i> -Hexane	29	67	2730b	1.3	6a/473		
<i>n</i> -Heptane							
<i>n</i> -Octane							
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP							
Cyclohexane							
Benzene				1.0	7/121		
Toluene							
Ethylbenzene							
Xylenes							
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	78	56	1923				
Ethanol							
<i>n</i> -Propanol							
<i>i</i> -Propanol							
<i>n</i> -Butanol				1.6	2f/123	0.11	V4/158
<i>i</i> -Butanol							
<i>s</i> -Butanol							
<i>n</i> -Amyl alc.							
<i>i</i> -Amyl alc.				24.8	2f/373		
Cyclohexanol							
1-Octanol							
Ethanediol							
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME							
EEE							
EGBE							
<i>Chlorinated</i>							
MDC							
Chloroform				1.0	1x/3/948		
Carbon tet.	Azeo			1.1	8/82		
1,2-EDC	None		2729	1.2	1x/3/948		
1,1,1-TCA	-		-	-	-	-	-
TCE				1.0	1x/3/948		
Perk.							
MCB							

Chlorinated solvents

Solute	Azeotrope		Reference	Solute $\gamma^{\sim}$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Ketones</i> Acetone MEK MIBK Cyclohexanone NMP Acetophenone							
<i>Ethers</i> Diethyl ether DIPE Dibutyl ether MTBE 1,4-Dioxane THF						0.04	V4/160
<i>Esters</i> Me acetate Et acetate <i>i</i> -Propyl acetate <i>n</i> -Butyl acetate Cellosolve acetate							
<i>Miscellaneous</i> DMF DMAc DMSO Sulfolane CS <sub>2</sub> Acetic acid Aniline Nitrobenzene Morpholine Pyridine 2-Nitropropane Acetonitrile Furfuraldehyde Phenol Water	96	65				0.04	V4/159



# Trichloroethylene

## Alternative names

1,2,2-trichloroethylene, trike, TCE, triclene, trilane, trichloroethene, **not** trichlorethane

## Reference codes

CAS number	79 01 6	Hazchem code	2Z
UN number	1710	EPA code	U228

## Physical properties

Molecular weight	131	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.17
Empirical formula	C <sub>2</sub> H <sub>1</sub> Cl <sub>3</sub>	Surface tension (@20°C dyn/cm)	29.5
Boiling point (°C)	87	Absolute viscosity (@25°C cP)	0.57
Freezing point (°C)	-86	Refractive index (25°C)	1.475
Specific gravity (20/4)	1.464		

## Fire hazards

Flash point (closed cup °C)	32*	Lower explosive limit (ppm)	80000
Autoignition temperature (°C)	420	Upper explosive limit (ppm)	105000
Electrical conductivity	8E-12		

## Health hazards

IDLH (ppm)	500	Vapour concentration @21°C ppm	80260
OES-TWA	100	Vapour density (relative to air)	4.55
OES-STEL	150	Vapour pressure @21°C mmHg	56.5
Odour threshold (ppm)	200	POCP	6.6

## Aqueous effluent

Solubility in water (25°C %w/w)	0.11
Solubility of water in (25°C %w/w)	0.033
Log <sub>10</sub> activated carbon partition	5.0
Log <sub>10</sub> partition in octanol/water (w/w)	+2.29
Biological oxygen demand w/w (days)	
Theoretical oxygen demand w/w	0.61

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	6.51827
	B	1018.603
	C	192.731

## Cox chart

	A
	B

## Solvent properties

Solubility parameter	8.0	Kauri butanol value	130
Dipole (D)	0.9	Evaporation time (ether = 1)	3.1
Dielectric constant (20°C)	3.42	Evaporation time (BuAc = 1)	4.9
Polarity (water 100)	16.0		

## Thermal information

Latent heat (cal/mol)	7467
Nett heat of combustion (kcal/gmol)	206
Specific heat (cal/mol/°C)	30
Critical pressure (MN/m <sup>2</sup> )	4.90
Critical temperature (K)	571
Latent heat of fusion (cal/mol)	
Van der Waals' volume	3.31
Van der Waals' surface area	2.86
Molar volume	90.01

\*Very resistant to flashing.

Solute	Azeotrope		Reference	Solute $\gamma^*$	Reference	Partition coefficient	Reference
	X% w/w	°C					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane	None		1482				
<i>n</i> -Hexane	None		2330	1.5	6a/463		
<i>n</i> -Heptane	None		2335				
<i>n</i> -Octane							
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP							
Cyclohexane	17	80	2328	1.3	6a/155		
Benzene	None		2326	1.0	7/114		
Toluene				0.8	7/370		
Ethylbenzene							
Xylenes							
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	62	59	1915	6.9	2a/40	8.9	V2/79
Ethanol	71	72	2286	7.3	2a/295	2.03	CEH
<i>n</i> -Propanol	83	82	2296	2.7	2a/518	0.24	V4/152
<i>i</i> -Propanol	70	75	2295	3.1	2d/43		
<i>n</i> -Butanol	97	87	2306	3.7	2f/121	0.08	V4/154
<i>i</i> -Butanol	91	85	2309				
<i>s</i> -Butanol	85	84	2307	3.8	2f/217		
<i>n</i> -Amyl alc.							
<i>i</i> -Amyl alc.	None		2321				
Cyclohexanol							
1-Octanol							
Ethanediol	None		2287				
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME							
EGME							
EEE							
EGBE							
<i>Chlorinated</i>							
MDC							
Chloroform				1.1	1x/3/943		
Carbon tet.	None		1093	1.0	1x/3/943		
1,2-EDC	33	82	2281	1.4	8/351		
1,1,1-TCA				1.0	1x/3/943		
TCE	-		-	-	-	-	-
Perk.				1.6	8/326		
MCB							

Chlorinated solvents

Solute	Azeotrope		Solute $\gamma^*$	Reference	Partition coefficient	Reference	
	X% w/w	°C					Reference
<i>Ketones</i>							
Acetone	None		1.0	3b/51	0.05	V2/157	
MEK	None	2289	1.3	3+4/264			
MIBK		2299	1.1	3b/517			
Cyclohexanone							
NMP							
Acetophenone							
<i>Ethers</i>							
Diethyl ether					0.05	V4/151	
DIPE	None	2331					
Dibutyl ether							
MTBE							
1,4-Dioxane	None	2301					
THF							
<i>Esters</i>							
Me acetate					0.6	5/575	
Et acetate	None	2302	1.0	5/454			
<i>i</i> -Propyl acetate	None	2317					
<i>n</i> -Butyl acetate			0.6	5/575			
Cellosolve acetate							
<i>Miscellaneous</i>							
DMF					2.7	V2/151	
DMAc							
DMSO							
Sulfolane							
CS <sup>2</sup>							
Acetic acid	96	86	2282	4.7			5/72
Aniline							
Nitrobenzene							
Morpholine							
Pyridine							
2-Nitropropane							
Acetonitrile	71	75	2280	5.5			8/349
Furfuraldehyde				3.1	3+4/37		
Phenol					0.03	V4/155	
Water	94	73	218				

# Perchloroethylene

## Alternative names

Tetrachloroethylene, perk, tetrachloroethene

## Reference codes

CAS number	127 18 4	Hazchem code	ZZ
UN number	1897	EPA code	U210

## Physical properties

Molecular weight	166	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	1.02
Empirical formula	C <sub>2</sub> Cl <sub>4</sub>	Surface tension (@20°C dyn/cm)	32
Boiling point (°C)	122	Absolute viscosity (@25°C cP)	0.88
Freezing point (°C)	-36	Refractive index (25°C)	1.504
Specific gravity (20/4)	1.63		

## Fire hazards

Flash point (closed cup °C)	None	Lower explosive limit (ppm)	None
Autoignition temperature (°C)	None	Upper explosive limit (ppm)	None
Electrical conductivity	5.5E-4		

## Health hazards

IDLH (ppm)	400	Vapour concentration @21°C ppm	20600
OES-TWA	50	Vapour density (relative to air)	5.8
OES-STEL	150	Vapour pressure @21°C mmHg	15.4
Odour threshold (ppm)	300	POCP	0.5

## Aqueous effluent

Solubility in water (25°C %w/w)	0.015
Solubility of water in (25°C %w/w)	0.0105
Log <sub>10</sub> activated carbon partition	5.4
Log <sub>10</sub> partition in octanol/water (w/w)	+2.60
Biological oxygen demand w/w (days)	0.06 (5)
Theoretical oxygen demand w/w	0.39

## Vapour pressure equation constants (Log<sub>10</sub>, mmHg)

Antoine equation	A	7.62930
	B	1803.96
	C	258.976

## Cox chart

	A
	B

## Solvent properties

Solubility parameter	4.5	Kauri butanol value	90
Dipole (D)	0	Evaporation time (ether = 1)	6.0
Dielectric constant (20°C)	2.3	Evaporation time (BuAc = 1)	2.6
Polarity (water 100)			

## Thermal information

Latent heat (cal/mol)	8316
Nett heat of combustion (kcal/gmol)	162
Specific heat (cal/mol/°C)	35
Critical pressure (MN/m <sup>2</sup> )	4.48
Critical temperature (K)	613
Latent heat of fusion (cal/mol)	
Van der Waals' volume	3.89
Van der Waals' surface area	3.40
Molar volume	101.84

Solute	Azeotrope		Reference	Solute $\gamma^{\circ}$	Reference	Partition coefficient	Reference
	X% w/w	$^{\circ}\text{C}$					
<i>Hydrocarbons</i>							
<i>n</i> -Pentane	None		2217a	1.5	6a/453		
<i>n</i> -Hexane	None						
<i>n</i> -Heptane							
<i>n</i> -Octane	92	120	2227				
<i>n</i> -Nonane							
<i>n</i> -Decane							
2,2,4-TMP							
Cyclohexane							
Benzene				1.3	7/112		
Toluene	None		2220				
Ethylbenzene	None		2225				
Xylenes	None		1167c				
C <sub>9</sub> Aromatics							
Tetralin							
<i>Alcohols</i>							
Methanol	36	64	1914	16.4	2a/37		
Ethanol	37	77	2162	5.4	2c/285		
<i>n</i> -Propanol	30	82	2176				
<i>i</i> -Propanol	52	94	2177	5.9	2d/42	2.6	CEH
<i>n</i> -Butanol	71	109	2186	3.8	2d/155		
<i>i</i> -Butanol	60	103	2189			21.7	CEH
<i>s</i> -Butanol	43	97	2187	3.3	2d/240		
<i>n</i> -Amyl alc.	85	117	2201				
<i>i</i> -Amyl alc.	81	116	2203				
Cyclohexanol							
1-Octanol							
Ethanediol	94	119	2163				
DEG							
1,2-Propanediol							
<i>Glycol ethers</i>							
PGME	95	121	2205				
EGME	76	110	2178				
EEE	84	116	2190				
EGBE	None		2218				
<i>Chlorinated</i>							
MDC				1.1	8/256		
Chloroform	None		1431	1.2	8/215		
Carbon tet.	None		1091	1.0	8/78		
1,2-EDC				2.0	8/340		
1,1,1-TCA							
TCE				1.1	8/327		
Perk.	-		-	-	-	-	-
MCB							

*Chlorinated solvents*

Solute	Azeotrope		Reference	Solute $\gamma^*$	Reference	Part coefficient	Reference
	X% w/w	°C					
<i>Ketones</i>							
Acetone	None		2168	2.6	3b/49	4.2	CEH
MEK							
MIBK	48	114	2209				
Cyclohexanone							
NMP							
Acetophenone							
<i>Ethers</i>							
Diethyl ether							
DIPE							
Dibutyl ether							
MTBE							
1,4-Dioxane	None		2181				
THF					0.08	V4/149	
<i>Esters</i>							
Me acetate							
Et acetate							
<i>i</i> -Propyl acetate							
<i>n</i> -Butyl acetate	79	120	2210				
Cellosolve acetate							
<i>Miscellaneous</i>							
DMF							
DMAc							
DMSO							
Sulfolane							
CS <sub>2</sub>				1.4	8.316		
Acetic acid	61	107	2158			7.25	V2/147
Aniline							
Nitrobenzene							
Morpholine							
Pyridine	52	113	2192	2.0	8/346		
2-Nitropropane							
Acetonitrile							
Furfuraldehyde	None		2191	4.3	3a/117	0.05	V4/150
Phenol							
Water	84	88	217				

# Monochlorobenzene

## Alternative names

Chlorobenzene, MCB, phenyl chloride

## Reference codes

CAS number	108 90 7	Hazchem code	2Y
UN number	1134	EPA code	U037

## Physical properties

Molecular weight	113	Cubic expansion coeff (per °C × 10 <sup>3</sup> )	0.98
Empirical formula	C <sub>6</sub> H <sub>5</sub> Cl <sub>1</sub>	Surface tension (@20°C dyn/cm)	33
Boiling point (°C)	132	Absolute viscosity (@25°C cP)	0.8
Freezing point (°C)	-46	Refractive index (25°C)	1.523
Specific gravity (20/4)	1.106		

## Fire hazards

Flash point (closed cup °C)	29	Lower explosive limit (ppm)	13000
Autoignition temperature (°C)	640	Upper explosive limit (ppm)	71000
Electrical conductivity	7E-11		

## Health hazards

IDLH (ppm)	2400	Vapour concentration @21°C ppm	12650
OES-TWA	50	Vapour density (relative to air)	3.9
OES-STEL		Vapour Pressure @21°C mmHg	9.5
Odour threshold (ppm)	1	POCP	

## Aqueous effluent

Solubility in water (25°C %w/w)	0.049
Solubility of water in (25°C %w/w)	0.033
Log <sub>10</sub> activated carbon partition	4.9
Log <sub>10</sub> partition in octanol/water (w/w)	+2.84
Biological oxygen demand w/w (days)	0.03 (5)
Theoretical oxygen demand w/w	2.05

## Vapour pressure equation constants (Log<sub>10</sub> mmHg)

Antoine equation	A	7.17294
	B	1549.200
	C	229.260
Cox chart	A	7.18576
	B	1558.4

## Solvent properties

Solubility parameter	9.5	Kauri butanol value	90
Dipole (D)	1.3	Evaporation time (ether = 1)	10.0
Dielectric constant (20°C)	5.62	Evaporation time (BuAc = 1)	
Polarity (water 100)	18.8		

## Thermal information

Latent heat (cal/mol)	8814
Nett heat of combustion (kcal/gmol)	754
Specific heat (cal/mol/°C)	35
Critical pressure (MN/m <sup>2</sup> )	4.52
Critical temperature (K)	632
Latent heat of fusion (cal/mol)	2305
Van der Waals' volume	3.81
Van der Waals' surface area	2.84
Molar volume	102.24

Solute	Azeotrope		Solute $\gamma^a$	Reference	Partition coefficient	Reference
	X% w/w	°C				
<i>Hydrocarbons</i>						
<i>n</i> -Pentane						
<i>n</i> -Hexane	None		1.6	6a/529		
<i>n</i> -Heptane	None		1.8	6b/119		
<i>n</i> -Octane	None		2.2	1x/3/1175		
<i>n</i> -Nonane						
<i>n</i> -Decane			1.5	6b/392		
2,2,4-TMP						
Cyclohexane	None		1.3	6a/202		
Benzene	None		1.0	7/243		
Toluene	None		1.0	7/416		
Ethylbenzene	None		1.0	7/469		
Xylenes	None		0.9	7/508		
<i>C<sub>9</sub> Aromatics</i>						
Tetralin						
<i>Alcohols</i>						
Methanol	None		4.9	2a/204		
Ethanol	None		4.2	2a/397		
<i>n</i> -Propanol	20	97	3.0	2a/552		
<i>i</i> -Propanol	None		3.4	2d/64		
<i>n</i> -Butanol	44	115	2.5	2b/175		
<i>i</i> -Butanol	37	107	2.8	2d/357		
<i>s</i> -Butanol	None		2.8	2b/258		
<i>n</i> -Amyl alc.	75	126				
<i>i</i> -Amyl alc.	66	124				
Cyclohexanol	None		2.6	2b/395		
1-Octanol						
Ethanediol	94	130				
DEG						
1,2-Propanediol						
<i>Glycol ethers</i>						
PGME	None					
EGME	53	119	3.4	2d/120		
EEE	68	127				
EGBE	None				0.16	P3988
<i>Chlorinated</i>						
MDC						
Chloroform	None		1.2	8/244		
Carbon tet.	None		1.2	8/166		
1,2-EDC						
1,1,1-TCA						
TCE						
Perk.						
MCB	-		-	-	-	-

Chlorinated solvents



Solute	Azeotrope		Solute $\gamma^*$	Reference	Partition coefficient	Reference
	X% w/w	°C				
<i>Ketones</i>						
Acetone	None		1.3	3+4/192	0.17	V2/477
MEK	None		1.3	3+4/283	0.08	V3/22
MIBK	None		1.1	3b/543		
Cyclohexanone	None					
NMP						
Acetophenone						
<i>Ethers</i>						
Diethyl ether						
DIPE						
Dibutyl ether	None					
MTBE						
1,4-Dioxane			0.9	1x/3/1175		
THF						
<i>Esters</i>						
Me acetate			1.2	5/374		
Et acetate	None		1.4	5/492		
<i>i</i> -Propyl acetate						
<i>n</i> -Butyl acetate	None					
Cellosolve acetate						
<i>Miscellaneous</i>						
DMF						
DMAc						
DMSO						
Sulfolane						
CS <sub>2</sub>						
Acetic acid	41	115			3.7	CEH
Aniline	None		1.8	8/527		
Nitrobenzene	None		1.1	1x/3/1175		
Morpholine						
Pyridine					0.08	V3/226
2-Nitropropane						
Acetonitrile	None		3.3	8/381	0.32	V2/176
Furfuraldehyde	None				0.01	V4/255
Phenol	None					
Water	72	90				