Benzene, (dichloromethyl)-

Other names:	(Dichloromethyl)benzene
	ALPHA,ALPHA-DICHLOROTOLUENE
	BENZAL CHLORIDE
	BENZYL DICHLORIDE
	Benzylene chloride
	Benzylidene chloride
	Benzylidene dichloride
	Chlorobenzal
	Chlorure de benzylidene
	Dichlorophenylmethane
	NSC 7915
	Rcra waste number U017
	Toluene, «alpha»,«alpha»-dichloro-
	Toluene, Â«alphaÂ»,Â«alphaÂ»-dichloro-
	UN 1886
	«alpha»,«alpha»-DichlorotoIuene
	«alpha»,«alpha»-Dichlorotoluene
	«alpha»,«alpha»-Dichlortoluene
	Â«alphaÂ»,Â«alphaÂ»-DichlorotoIuene
	Â«alphaÂ»,Â«alphaÂ»-Dichlorotoluene
	Â«alphaÂ»,Â«alphaÂ»-Dichlortoluene
Inchi:	InChI=1S/C7H6Cl2/c8-7(9)6-4-2-1-3-5-6/h1-5,7H
InchiKey:	CAHQGWAXKLQREW-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	ClC(Cl)c1ccccc1
Mol. weight [g/mol]:	161.03
CAS:	98-87-3

Physical Properties

Property code	Value	Unit	Source
gf	94.17	kJ/mol	Joback Method
hf	11.96	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.163		Crippen Method

mcvol	110.210	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1108.20		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1672.00		NIST Webbook
tb	450.30 ± 0.15	K	NIST Webbook
tc	692.87	K	Joback Method
tf	256.20 ± 0.50	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.75	J/mol×K	692.87	Joback Method
cpg	232.64	J/mol×K	654.16	Joback Method
cpg	224.90	J/mol×K	615.46	Joback Method
cpg	216.51	J/mol×K	576.76	Joback Method
cpg	207.42	J/mol×K	538.06	Joback Method
cpg	197.59	J/mol×K	499.36	Joback Method
cpg	186.98	J/mol×K	460.66	Joback Method
dvisc	0.0045487	Pa×s	239.91	Joback Method
dvisc	0.0002869	Pa×s	460.66	Joback Method
dvisc	0.0003724	Pa×s	423.87	Joback Method
dvisc	0.0005078	Pa×s	387.08	Joback Method
dvisc	0.0007392	Pa×s	350.29	Joback Method
dvisc	0.0011751	Pa×s	313.49	Joback Method
dvisc	0.0021130	Pa×s	276.70	Joback Method
hvapt	49.50	kJ/mol	397.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.87285e+01
Coeff. B	-5.91063e+03
Coeff. C	-3.14080e+01
Temperature range (K), min.	351.93
Temperature range (K), max.	471.94

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.81017e+01
Coeff. B	-7.18848e+03
Coeff. C	-4.71346e+00
Coeff. D	1.86704e-06
Temperature range (K), min.	257.00
Temperature range (K), max.	731.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1696
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1696.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98873&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume