1,3-DICHLORO-2-(METHOXYMETHYL)BENZENE

Other names: Benzene, 1,3-dichloro-2-(methoxymethyl)-
2,6-Dichlorobenzyl alcohol, methyl ether
1,3-Dichloro-2-(methoxymethyl)benzene
Inchi: InChI=1S/C8H8Cl2O/c1-11-5-6-7(9)3-2-4-8(6)10/h2-4H,5H2,1H3
InchiKey: QBKBHXIQLAMKOB-UHFFFAOYSA-N
Formula: C8H8Cl2O
SMILES: COCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 191.06

Physical Properties

Property code	Value	Unit	Source
hfus	19.32	kJ/mol	Joback Method
hvap	60.98	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	3.140		Crippen Method
mcvol	130.170	ml/mol	McGowan Method
rinpol	1342.00		NIST Webbook
rinpol	1342.00		NIST Webbook
tb	503.98	K	Cheméo Relay (1.0)
tf	324.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.81	J/mol×K	516.36	Joback Method
cpg	258.26	J/mol×K	553.54	Joback Method
cpg	268.15	J/mol×K	590.71	Joback Method
cpg	277.50	J/mol×K	627.89	Joback Method
cpg	286.30	J/mol×K	665.07	Joback Method
cpg	294.58	J/mol×K	702.24	Joback Method
cpg	302.33	J/mol×K	739.42	Joback Method
dvisc	0.0013663	Pa×s	313.45	Joback Method
dvisc	0.0008682	Pa×s	347.27	Joback Method

dvisc	0.0005980	Pa×s	381.09	Joback Method
dvisc	0.0004376	Pa×s	414.91	Joback Method
dvisc	0.0003357	Pa×s	448.72	Joback Method
dvisc	0.0002673	Pa×s	482.54	Joback Method
dvisc	0.0002193	Pa×s	516.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33486907&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point