2,6-Dichlorobenzyl methyl ether

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
CAS: 33486-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-19.23	kJ/mol	Joback Method
hf	-158.56	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	48.18	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.140		Crippen Method
mcvol	130.170	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1342.00		NIST Webbook
tb	516.36	K	Joback Method
tc	739.42	K	Joback Method
tf	313.45	K	Joback Method
vc	0.491	m3/kmol	Joback Method

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	414.90	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

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33486907&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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