Benzenemethanol, 2,4-dichloro-«alpha»-(chloromethyl)-

Other names: Benzyl alcohol, 2,4-dichloro-«alpha»-(chloromethyl)-
2-Chloro-1-(2,4-dichlorophenyl)ethanol
2,4-Dichloro-«alpha»-(chloromethyl)benzyl alcohol
«alpha»-(2,4-Dichlorophenyl)-«beta»-chloroethanol
«alpha»-(Chloromethyl)-2,4-dichlorobenzyl alcohol

Inchi: InChI=1S/C8H7Cl3O/c9-4-8(12)6-2-1-5(10)3-7(6)11/h1-3,8,12H,4H2

InchiKey: XHEPANNURIQWRM-UHFFFAOYSA-N

Formula: C8H7Cl3O

SMILES: OC(CCl)c1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 225.50

CAS: 13692-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-65.42	kJ/mol	Joback Method
hf	-199.59	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.266		Crippen Method
mcvol	142.410	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	623.11	K	Joback Method
tc	840.14	K	Joback Method
tf	366.96	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.41	J/mol×K	623.11	Joback Method
cpg	325.23	J/mol×K	803.97	Joback Method
cpg	319.08	J/mol×K	767.80	Joback Method
cpg	312.44	J/mol×K	731.62	Joback Method

cpg	305.31	J/mol×K	695.45	Joback Method
cpg	297.64	J/mol×K	659.28	Joback Method
cpg	330.94	J/mol×K	840.14	Joback Method
dvisc	0.0000808	Pa×s	623.11	Joback Method
dvisc	0.0001188	Pa×s	580.42	Joback Method
dvisc	0.0001858	Pa×s	537.73	Joback Method
dvisc	0.0003137	Pa×s	495.04	Joback Method
dvisc	0.0005846	Pa×s	452.34	Joback Method
dvisc	0.0012407	Pa×s	409.65	Joback Method
dvisc	0.0031368	Pa×s	366.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13692143&Units=SI
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume