

2,6-Dichlorobenzyl alcohol, 2-methylpropyl ether

Inchi:	InChI=1S/C11H14Cl2O/c1-8(2)6-14-7-9-10(12)4-3-5-11(9)13/h3-5,8H,6-7H2,1-2H3
InchiKey:	KVOKIMTYAZWXAE-UHFFFAOYSA-N
Formula:	C11H14Cl2O
SMILES:	CC(C)COCc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	233.13

Physical Properties

Property code	Value	Unit	Source
gf	3.59	kJ/mol	Joback Method
hf	-225.76	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.166		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	584.56	K	Joback Method
tc	800.88	K	Joback Method
tf	332.26	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.37	J/mol×K	584.56	Joback Method
cpg	396.17	J/mol×K	620.61	Joback Method
cpg	409.20	J/mol×K	656.67	Joback Method
cpg	421.48	J/mol×K	692.72	Joback Method
cpg	433.01	J/mol×K	728.77	Joback Method
cpg	443.83	J/mol×K	764.82	Joback Method
cpg	453.94	J/mol×K	800.88	Joback Method
dvisc	0.0016170	Pa×s	332.26	Joback Method

dvisc	0.0008859	Pa×s	374.31	Joback Method
dvisc	0.0005481	Pa×s	416.36	Joback Method
dvisc	0.0003703	Pa×s	458.41	Joback Method
dvisc	0.0002672	Pa×s	500.46	Joback Method
dvisc	0.0002029	Pa×s	542.51	Joback Method
dvisc	0.0001602	Pa×s	584.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378127&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

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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