

2,6-Dichlorobenzyl alcohol, 1-methylpropyl ether

Inchi:	InChI=1S/C11H14Cl2O/c1-3-8(2)14-7-9-10(12)5-4-6-11(9)13/h4-6,8H,3,7H2,1-2H3
InchiKey:	BSOUAKGVMFUNNY-UHFFFAOYSA-N
Formula:	C11H14Cl2O
SMILES:	CCC(C)OCc1c(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	-4.59		Crippen Method
logp	4.308		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinsol	1531.00		NIST Webbook
tb	584.56	K	Joback Method
tc	800.88	K	Joback Method
tf	332.26	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.37	J/molxK	584.56	Joback Method
cpg	443.83	J/molxK	764.82	Joback Method
cpg	433.01	J/molxK	728.77	Joback Method
cpg	421.48	J/molxK	692.72	Joback Method
cpg	409.20	J/molxK	656.67	Joback Method
cpg	396.17	J/molxK	620.61	Joback Method
cpg	453.94	J/molxK	800.88	Joback Method
dvisc	0.0001602	Paxs	584.56	Joback Method
dvisc	0.0002029	Paxs	542.51	Joback Method

dvisc	0.0002672	Paxs	500.46	Joback Method
dvisc	0.0003703	Paxs	458.41	Joback Method
dvisc	0.0005481	Paxs	416.36	Joback Method
dvisc	0.0008859	Paxs	374.31	Joback Method
dvisc	0.0016170	Paxs	332.26	Joback Method

Sources

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=U378131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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