

2,3-Dichlorobenzyl alcohol, n-butyl ether

Inchi:	InChI=1S/C11H14Cl2O/c1-2-3-7-14-8-9-5-4-6-10(12)11(9)13/h4-6H,2-3,7-8H2,1H3
InchiKey:	KYIRIZHXJQXZGC-UHFFFAOYSA-N
Formula:	C11H14Cl2O
SMILES:	CCCCOCc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	233.13

Physical Properties

Property code	Value	Unit	Source
gf	6.03	kJ/mol	Joback Method
hf	-220.48	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.310		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinsol	1640.00		NIST Webbook
tb	585.00	K	Joback Method
tc	796.84	K	Joback Method
tf	347.26	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.96	J/molxK	585.00	Joback Method
cpg	395.42	J/molxK	620.31	Joback Method
cpg	408.15	J/molxK	655.61	Joback Method
cpg	420.17	J/molxK	690.92	Joback Method
cpg	431.48	J/molxK	726.23	Joback Method
cpg	442.12	J/molxK	761.53	Joback Method
cpg	452.09	J/molxK	796.84	Joback Method
dvisc	0.0013156	Paxs	347.26	Joback Method
dvisc	0.0007871	Paxs	386.88	Joback Method

dvisc	0.0005181	Paxs	426.51	Joback Method
dvisc	0.0003661	Paxs	466.13	Joback Method
dvisc	0.0002732	Paxs	505.75	Joback Method
dvisc	0.0002127	Paxs	545.38	Joback Method
dvisc	0.0001713	Paxs	585.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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