

2,5-Dichlorobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H14Cl2O/c1-2-3-6-14-8-9-7-10(12)4-5-11(9)13/h4-5,7H,2-3,6,8H2,1H3
InchiKey: ZQHXBGQPYBLWEU-UHFFFAOYSA-N
Formula: C11H14Cl2O
SMILES: CCCCOCc1cc(Cl)ccc1Cl
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
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	585.00	K	Joback Method
tc	796.84	K	Joback Method
tf	347.26	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.96	J/mol×K	585.00	Joback Method
cpg	442.12	J/mol×K	761.53	Joback Method
cpg	431.48	J/mol×K	726.23	Joback Method
cpg	420.17	J/mol×K	690.92	Joback Method
cpg	408.15	J/mol×K	655.61	Joback Method
cpg	395.42	J/mol×K	620.31	Joback Method
cpg	452.09	J/mol×K	796.84	Joback Method
dvisc	0.0001713	Pa×s	585.00	Joback Method

dvisc	0.0002127	Pa×s	545.38	Joback Method
dvisc	0.0002732	Pa×s	505.75	Joback Method
dvisc	0.0003661	Pa×s	466.13	Joback Method
dvisc	0.0005181	Pa×s	426.51	Joback Method
dvisc	0.0007871	Pa×s	386.88	Joback Method
dvisc	0.0013156	Pa×s	347.26	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=U378119&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
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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