2,6-Dichlorobenzyl alcohol, 3-methylbutyl ether

Inchi: InChI=1S/C12H16Cl2O/c1-9(2)6-7-15-8-10-11(13)4-3-5-12(10)14/h3-5,9H,6-8H2,1-2H3
InchiKey: VAKZFBPIHZUVOA-UHFFFAOYSA-N
Formula: C12H16Cl2O
SMILES: CC(C)CCOCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 247.16

Physical Properties

Property code	Value	Unit	Source
gf	12.01	kJ/mol	Joback Method
hf	-246.40	kJ/mol	Joback Method
hfus	26.16	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.556		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	607.44	K	Joback Method
tc	820.11	K	Joback Method
tf	343.53	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.61	J/mol×K	607.44	Joback Method
cpg	445.15	J/mol×K	642.88	Joback Method
cpg	458.88	J/mol×K	678.33	Joback Method
cpg	471.81	J/mol×K	713.77	Joback Method
cpg	483.97	J/mol×K	749.22	Joback Method
cpg	495.37	J/mol×K	784.66	Joback Method
cpg	506.02	J/mol×K	820.11	Joback Method
dvisc	0.0015502	Pa×s	343.53	Joback Method
dvisc	0.0008347	Pa×s	387.51	Joback Method

dvisc	0.0005098	Pa×s	431.50	Joback Method
dvisc	0.0003412	Pa×s	475.49	Joback Method
dvisc	0.0002444	Pa×s	519.47	Joback Method
dvisc	0.0001844	Pa×s	563.46	Joback Method
dvisc	0.0001449	Pa×s	607.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378133&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
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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