

3,5-Dichlorobenzyl alcohol, 3-methylbutyl ether

Inchi:	InChI=1S/C12H16Cl2O/c1-9(2)3-4-15-8-10-5-11(13)7-12(14)6-10/h5-7,9H,3-4,8H2,1-2H1
InchiKey:	XONHVMYZERTNLX-UHFFFAOYSA-N
Formula:	C12H16Cl2O
SMILES:	CC(C)CCOCc1cc(Cl)cc(Cl)c1
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
mvol	186.530	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1665.00		NIST Webbook
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tb	607.44	K	Joback Method
tc	820.11	K	Joback Method
tf	343.53	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.61	J/molxK	607.44	Joback Method
cpg	445.15	J/molxK	642.88	Joback Method
cpg	458.88	J/molxK	678.33	Joback Method
cpg	471.81	J/molxK	713.77	Joback Method
cpg	483.97	J/molxK	749.22	Joback Method
cpg	495.37	J/molxK	784.66	Joback Method
cpg	506.02	J/molxK	820.11	Joback Method
dvisc	0.0015502	Paxs	343.53	Joback Method

dvisc	0.0008347	Paxs	387.51	Joback Method
dvisc	0.0005098	Paxs	431.50	Joback Method
dvisc	0.0003412	Paxs	475.49	Joback Method
dvisc	0.0002444	Paxs	519.47	Joback Method
dvisc	0.0001844	Paxs	563.46	Joback Method
dvisc	0.0001449	Paxs	607.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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