

2,3-Dichlorobenzyl alcohol, neopentyl ether

Inchi:	InChI=1S/C12H16Cl2O/c1-12(2,3)8-15-7-9-5-4-6-10(13)11(9)14/h4-6H,7-8H2,1-3H3
InchiKey:	FLNWRXZAZBAORY-UHFFFAOYSA-N
Formula:	C12H16Cl2O
SMILES:	CC(C)(C)COCc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	247.16

Physical Properties

Property code	Value	Unit	Source
gf	17.29	kJ/mol	Joback Method
hf	-249.87	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.556		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	604.65	K	Joback Method
tc	825.49	K	Joback Method
tf	360.95	K	Joback Method
vc	0.705	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.51	J/molxK	604.65	Joback Method
cpg	448.45	J/molxK	641.46	Joback Method
cpg	462.43	J/molxK	678.26	Joback Method
cpg	475.50	J/molxK	715.07	Joback Method
cpg	487.69	J/molxK	751.88	Joback Method
cpg	499.05	J/molxK	788.68	Joback Method
cpg	509.62	J/molxK	825.49	Joback Method
dvisc	0.0014004	Paxs	360.95	Joback Method

dvisc	0.0007826	Paxs	401.57	Joback Method
dvisc	0.0004867	Paxs	442.18	Joback Method
dvisc	0.0003279	Paxs	482.80	Joback Method
dvisc	0.0002348	Paxs	523.42	Joback Method
dvisc	0.0001765	Paxs	564.03	Joback Method
dvisc	0.0001378	Paxs	604.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375301&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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