

2,3-Dichlorobenzyl alcohol, n-pentyl ether

Inchi:	InChI=1S/C12H16Cl2O/c1-2-3-4-8-15-9-10-6-5-7-11(13)12(10)14/h5-7H,2-4,8-9H2,1H3
InchiKey:	PKYGCJGTLHRGKZ-UHFFFAOYSA-N
Formula:	C12H16Cl2O
SMILES:	CCCCCOCc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	247.16

Physical Properties

Property code	Value	Unit	Source
gf	14.45	kJ/mol	Joback Method
hf	-241.12	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.700		Crippen Method
mvol	186.530	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1745.00		NIST Webbook
tb	607.88	K	Joback Method
tc	816.32	K	Joback Method
tf	358.53	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.18	J/molxK	607.88	Joback Method
cpg	444.38	J/molxK	642.62	Joback Method
cpg	457.81	J/molxK	677.36	Joback Method
cpg	470.49	J/molxK	712.10	Joback Method
cpg	482.43	J/molxK	746.84	Joback Method
cpg	493.65	J/molxK	781.58	Joback Method
cpg	504.17	J/molxK	816.32	Joback Method
dvisc	0.0012696	Paxs	358.53	Joback Method
dvisc	0.0007459	Paxs	400.09	Joback Method

dvisc	0.0004843	Paxs	441.65	Joback Method
dvisc	0.0003387	Paxs	483.20	Joback Method
dvisc	0.0002507	Paxs	524.76	Joback Method
dvisc	0.0001939	Paxs	566.32	Joback Method
dvisc	0.0001554	Paxs	607.88	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=U375302&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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