

3,5-Dichlorobenzyl alcohol, isopropyl ether

Inchi:	InChI=1S/C10H12Cl2O/c1-7(2)13-6-8-3-9(11)5-10(12)4-8/h3-5,7H,6H2,1-2H3
InchiKey:	FZJKANNIOSZUDU-UHFFFAOYSA-N
Formula:	C10H12Cl2O
SMILES:	CC(C)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	219.11

Physical Properties

Property code	Value	Unit	Source
gf	-4.83	kJ/mol	Joback Method
hf	-205.12	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	52.25	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.918		Crippen Method
mvol	158.350	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1459.00		NIST Webbook
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tb	561.68	K	Joback Method
tc	781.85	K	Joback Method
tf	320.99	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.81	J/molxK	561.68	Joback Method
cpg	348.74	J/molxK	598.38	Joback Method
cpg	360.96	J/molxK	635.07	Joback Method
cpg	372.47	J/molxK	671.77	Joback Method
cpg	383.28	J/molxK	708.46	Joback Method
cpg	393.42	J/molxK	745.16	Joback Method
cpg	402.89	J/molxK	781.85	Joback Method
dvisc	0.0016690	Paxs	320.99	Joback Method

dvisc	0.0009314	Paxs	361.11	Joback Method
dvisc	0.0005841	Paxs	401.22	Joback Method
dvisc	0.0003987	Paxs	441.33	Joback Method
dvisc	0.0002900	Paxs	481.45	Joback Method
dvisc	0.0002216	Paxs	521.56	Joback Method
dvisc	0.0001759	Paxs	561.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378137&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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