

3,5-Dichlorobenzyl alcohol, tert.-butyl ether

Inchi:	InChI=1S/C11H14Cl2O/c1-11(2,3)14-7-8-4-9(12)6-10(13)5-8/h4-6H,7H2,1-3H3
InchiKey:	KXAGGFMQGVZDG-UHFFFAOYSA-N
Formula:	C11H14Cl2O
SMILES:	CC(C)(C)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	233.13

Physical Properties

Property code	Value	Unit	Source
gf	8.87	kJ/mol	Joback Method
hf	-229.23	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.308		Crippen Method
mvol	172.440	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	581.77	K	Joback Method
tc	806.74	K	Joback Method
tf	349.68	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.44	J/molxK	581.77	Joback Method
cpg	447.75	J/molxK	769.24	Joback Method
cpg	436.98	J/molxK	731.75	Joback Method
cpg	425.41	J/molxK	694.25	Joback Method
cpg	412.99	J/molxK	656.76	Joback Method
cpg	399.68	J/molxK	619.26	Joback Method
cpg	457.75	J/molxK	806.74	Joback Method
dvisc	0.0001544	Paxs	581.77	Joback Method

dvisc	0.0001968	Paxs	543.09	Joback Method
dvisc	0.0002604	Paxs	504.41	Joback Method
dvisc	0.0003609	Paxs	465.73	Joback Method
dvisc	0.0005307	Paxs	427.04	Joback Method
dvisc	0.0008427	Paxs	388.36	Joback Method
dvisc	0.0014821	Paxs	349.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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