2,4-Dichlorobenzyl alcohol, tert.-butyl ether

Inchi: InChI=1S/C11H14Cl2O/c1-11(2,3)14-7-8-4-5-9(12)6-10(8)13/h4-6H,7H2,1-3H3
InchiKey: MLNXVFOOJYBTEO-UHFFFAOYSA-N
Formula: C11H14Cl2O
SMILES: CC(C)(C)OCc1ccc(Cl)cc1Cl
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
mcvol	172.440	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		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/mol×K	581.77	Joback Method
cpg	399.68	J/mol×K	619.26	Joback Method
cpg	412.99	J/mol×K	656.76	Joback Method
cpg	425.41	J/mol×K	694.25	Joback Method
cpg	436.98	J/mol×K	731.75	Joback Method
cpg	447.75	J/mol×K	769.24	Joback Method
cpg	457.75	J/mol×K	806.74	Joback Method
dvisc	0.0014821	Pa×s	349.68	Joback Method

dvisc	0.0008427	Pa×s	388.36	Joback Method
dvisc	0.0005307	Pa×s	427.04	Joback Method
dvisc	0.0003609	Pa×s	465.73	Joback Method
dvisc	0.0002604	Pa×s	504.41	Joback Method
dvisc	0.0001968	Pa×s	543.09	Joback Method
dvisc	0.0001544	Pa×s	581.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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