2,4,6-Trichlorobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H13Cl3O/c1-7(2)5-15-6-9-10(13)3-8(12)4-11(9)14/h3-4,7H,5-6H2,1-2H3
InchiKey: DDQQMOKLWNGIOC-UHFFFAOYSA-N
Formula: C11H13Cl3O
SMILES: CC(C)COCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 267.58

Physical Properties

Property code	Value	Unit	Source
gf	-17.97	kJ/mol	Joback Method
hf	-252.97	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.819		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	626.97	K	Joback Method
tc	847.93	K	Joback Method
tf	374.70	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/mol×K	626.97	Joback Method
cpg	419.80	J/mol×K	663.80	Joback Method
cpg	431.76	J/mol×K	700.62	Joback Method
cpg	443.00	J/mol×K	737.45	Joback Method
cpg	453.51	J/mol×K	774.28	Joback Method
cpg	463.32	J/mol×K	811.10	Joback Method
cpg	472.44	J/mol×K	847.93	Joback Method
dvisc	0.0011413	Pa×s	374.70	Joback Method

dvisc	0.0006843	Pa×s	416.75	Joback Method
dvisc	0.0004506	Pa×s	458.79	Joback Method
dvisc	0.0003183	Pa×s	500.84	Joback Method
dvisc	0.0002373	Pa×s	542.88	Joback Method
dvisc	0.0001845	Pa×s	584.92	Joback Method
dvisc	0.0001484	Pa×s	626.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375280&Units=SI

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