2,4,6-Trichlorobenzyl alcohol, ethyl ether

Inchi: InChI=1S/C9H9Cl3O/c1-2-13-5-7-8(11)3-6(10)4-9(7)12/h3-4H,2,5H2,1H3
InchiKey: ICLBRTXAPUWKGI-UHFFFAOYSA-N
Formula: C9H9Cl3O
SMILES: CCOCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 239.53

Physical Properties

Property code	Value	Unit	Source
gf	-32.37	kJ/mol	Joback Method
hf	-206.41	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.183		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1527.00		NIST Webbook
tb	581.65	K	Joback Method
tc	806.16	K	Joback Method
tf	367.16	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.26	J/mol×K	581.65	Joback Method
cpg	323.87	J/mol×K	619.07	Joback Method
cpg	333.89	J/mol×K	656.49	Joback Method
cpg	343.33	J/mol×K	693.90	Joback Method
cpg	352.18	J/mol×K	731.32	Joback Method
cpg	360.47	J/mol×K	768.74	Joback Method
cpg	368.18	J/mol×K	806.16	Joback Method
dvisc	0.0010425	Pa×s	367.16	Joback Method

dvisc	0.0006957	Pa×s	402.91	Joback Method
dvisc	0.0004959	Pa×s	438.66	Joback Method
dvisc	0.0003720	Pa×s	474.41	Joback Method
dvisc	0.0002905	Pa×s	510.15	Joback Method
dvisc	0.0002344	Pa×s	545.90	Joback Method
dvisc	0.0001941	Pa×s	581.65	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=U375281&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