2,4,6-Trichlorobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H13Cl3O/c1-2-3-4-15-7-9-10(13)5-8(12)6-11(9)14/h5-6H,2-4,7H2,1H3
InchiKey: ZGVMKDVHCBPEGY-UHFFFAOYSA-N
Formula: C11H13Cl3O
SMILES: CCCCOCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 267.58

Physical Properties

Property code	Value	Unit	Source
gf	-15.53	kJ/mol	Joback Method
hf	-247.69	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.964		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	627.41	K	Joback Method
tc	843.95	K	Joback Method
tf	389.70	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.60	J/mol×K	627.41	Joback Method
cpg	419.01	J/mol×K	663.50	Joback Method
cpg	430.71	J/mol×K	699.59	Joback Method
cpg	441.73	J/mol×K	735.68	Joback Method
cpg	452.07	J/mol×K	771.77	Joback Method
cpg	461.74	J/mol×K	807.86	Joback Method
cpg	470.76	J/mol×K	843.95	Joback Method
dvisc	0.0009743	Pa×s	389.70	Joback Method

dvisc	0.0006269	Pa×s	429.32	Joback Method
dvisc	0.0004346	Pa×s	468.94	Joback Method
dvisc	0.0003190	Pa×s	508.56	Joback Method
dvisc	0.0002448	Pa×s	548.17	Joback Method
dvisc	0.0001947	Pa×s	587.79	Joback Method
dvisc	0.0001594	Pa×s	627.41	Joback Method

Sources

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=U375276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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