2,4,6-Trichlorobenzyl alcohol, 3-methylbutyl ether

Inchi: InChI=1S/C12H15Cl3O/c1-8(2)3-4-16-7-10-11(14)5-9(13)6-12(10)15/h5-6,8H,3-4,7H2,1-

InchiKey: VGFVUBFYUOTIAV-UHFFFAOYSA-N

Formula: C12H15Cl3O

SMILES: CC(C)CCOCc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 281.61

Physical Properties

Property code	Value	Unit	Source
gf	-9.55	kJ/mol	Joback Method
hf	-273.61	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.210		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1771.00		NIST Webbook
tb	649.85	K	Joback Method
tc	866.96	K	Joback Method
tf	385.97	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.19	J/mol×K	649.85	Joback Method
cpg	515.57	J/mol×K	830.78	Joback Method
cpg	505.21	J/mol×K	794.59	Joback Method
cpg	494.11	J/mol×K	758.41	Joback Method
cpg	482.25	J/mol×K	722.22	Joback Method
cpg	469.61	J/mol×K	686.04	Joback Method
cpg	525.21	J/mol×K	866.96	Joback Method
dvisc	0.0001330	Pa×s	649.85	Joback Method
dvisc	0.0001662	Pa×s	605.87	Joback Method

dvisc	0.0002150	Pa×s	561.89	Joback Method
dvisc	0.0002906	Pa×s	517.91	Joback Method
dvisc	0.0004154	Pa×s	473.93	Joback Method
dvisc	0.0006387	Pa×s	429.95	Joback Method
dvisc	0.0010834	Pa×s	385.97	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=U375273&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