2-Chloro-6-fluorobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H14ClFO/c1-8(2)6-14-7-9-10(12)4-3-5-11(9)13/h3-5,8H,6-7H2,1-2H3
InchiKey: USRZSMBUILAMOK-UHFFFAOYSA-N
Formula: C11H14ClFO
SMILES: CC(C)COCc1c(F)cccc1Cl
Mol. weight [g/mol]: 216.68

Physical Properties

Property code	Value	Unit	Source
gf	-179.29	kJ/mol	Joback Method
hf	-406.13	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.652		Crippen Method
mcvol	161.970	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1358.00		NIST Webbook
tb	546.40	K	Joback Method
tc	748.23	K	Joback Method
tf	302.93	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.48	J/mol×K	546.40	Joback Method
cpg	377.37	J/mol×K	580.04	Joback Method
cpg	390.57	J/mol×K	613.68	Joback Method
cpg	403.09	J/mol×K	647.32	Joback Method
cpg	414.94	J/mol×K	680.96	Joback Method
cpg	426.14	J/mol×K	714.60	Joback Method
cpg	436.70	J/mol×K	748.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378143&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
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