3,4,5-Trifluorobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H13F3O/c1-7(2)5-15-6-8-3-9(12)11(14)10(13)4-8/h3-4,7H,5-6H2,1-2H3
InchiKey: AHJQKSXPNFZNEA-UHFFFAOYSA-N
Formula: C11H13F3O
SMILES: CC(C)COCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 218.22

Physical Properties

Property code	Value	Unit	Source
gf	-566.61	kJ/mol	Joback Method
hf	-794.08	kJ/mol	Joback Method
hfus	24.03	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.276		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1210.00		NIST Webbook
tb	512.49	K	Joback Method
tc	692.17	K	Joback Method
tf	286.71	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.76	J/mol×K	512.49	Joback Method
cpg	364.68	J/mol×K	542.44	Joback Method
cpg	377.06	J/mol×K	572.38	Joback Method
cpg	388.92	J/mol×K	602.33	Joback Method
cpg	400.27	J/mol×K	632.28	Joback Method
cpg	411.10	J/mol×K	662.22	Joback Method
cpg	421.43	J/mol×K	692.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375250&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

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