2,3,4,5-Tetrafluorobenzyl alcohol, 1-methylpropyl ether

Inchi: InChI=1S/C11H12F4O/c1-3-6(2)16-5-7-4-8(12)10(14)11(15)9(7)13/h4,6H,3,5H2,1-2H3

InchiKey: KDNBLDQUQZZDIQ-UHFFFAOYSA-N

Formula: C11H12F4O

SMILES: CCC(C)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 236.21

Physical Properties

Property code	Value	Unit	Source
gf	-771.05	kJ/mol	Joback Method
hf	-1001.66	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.558		Crippen Method
mcvol	155.040	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	516.74	K	Joback Method
tc	689.33	K	Joback Method
tf	299.82	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.23	J/mol×K	516.74	Joback Method
cpg	372.28	J/mol×K	545.51	Joback Method
cpg	383.87	J/mol×K	574.27	Joback Method
cpg	395.01	J/mol×K	603.04	Joback Method
cpg	405.69	J/mol×K	631.80	Joback Method
cpg	415.93	J/mol×K	660.57	Joback Method
cpg	425.72	J/mol×K	689.33	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=U375295&Units=SI

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