1-(2-Methoxyethoxy)-2-methyl-2-propanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H15ClF2O4/c1-8(2,6-15-5-4-14-3)16-7(13)9(10,11)12/h4-6H2,1-3H3
InchiKey: GJRKNSCSZBFCQD-UHFFFAOYSA-N
Formula: C9H15ClF2O4
SMILES: COCCOCC(C)(C)OC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 260.66

Physical Properties

Property code	Value	Unit	Source
gf	-814.89	kJ/mol	Joback Method
hf	-1163.79	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.803		Crippen Method
mcvol	172.630	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	555.96	K	Joback Method
tc	736.56	K	Joback Method
tf	343.75	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.93	J/mol×K	555.96	Joback Method
cpg	437.71	J/mol×K	586.06	Joback Method
cpg	449.83	J/mol×K	616.16	Joback Method
cpg	461.32	J/mol×K	646.26	Joback Method
cpg	472.18	J/mol×K	676.36	Joback Method
cpg	482.44	J/mol×K	706.46	Joback Method
cpg	492.11	J/mol×K	736.56	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=U376273&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