5-Methyl-2-hexanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H15ClF2O2/c1-6(2)4-5-7(3)14-8(13)9(10,11)12/h6-7H,4-5H2,1-3H3
InchiKey: RHZQAYIXTJYXHY-UHFFFAOYSA-N
Formula: C9H15ClF2O2
SMILES: CC(C)CCC(C)OC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 228.66

Physical Properties

Property code	Value	Unit	Source
gf	-612.61	kJ/mol	Joback Method
hf	-901.16	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.186		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook
tb	513.47	K	Joback Method
tc	692.98	K	Joback Method
tf	266.87	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.29	J/mol×K	513.47	Joback Method
cpg	385.42	J/mol×K	543.39	Joback Method
cpg	397.90	J/mol×K	573.31	Joback Method
cpg	409.75	J/mol×K	603.22	Joback Method
cpg	420.97	J/mol×K	633.14	Joback Method
cpg	431.60	J/mol×K	663.06	Joback Method
cpg	441.66	J/mol×K	692.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376271&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