2,2-Dimethyl-3-pentanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H15ClF2O2/c1-5-6(8(2,3)4)14-7(13)9(10,11)12/h6H,5H2,1-4H3
InchiKey: AQMSWNKBTGSBHG-UHFFFAOYSA-N
Formula: C9H15ClF2O2
SMILES: CCC(OC(=O)C(F)(F)Cl)C(C)(C)C
Mol. weight [g/mol]: 228.66

Physical Properties

Property code	Value	Unit	Source
gf	-607.33	kJ/mol	Joback Method
hf	-904.63	kJ/mol	Joback Method
hfus	13.86	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.186		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	510.68	K	Joback Method
tc	696.92	K	Joback Method
tf	284.29	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.15	J/mol×K	510.68	Joback Method
cpg	388.91	J/mol×K	541.72	Joback Method
cpg	401.87	J/mol×K	572.76	Joback Method
cpg	414.06	J/mol×K	603.80	Joback Method
cpg	425.51	J/mol×K	634.84	Joback Method
cpg	436.26	J/mol×K	665.88	Joback Method
cpg	446.34	J/mol×K	696.92	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=U376264&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