«beta»-Citronellol, chlorodifluoroacetate

Inchi: InChI=1S/C12H19ClF2O2/c1-9(2)5-4-6-10(3)7-8-17-11(16)12(13,14)15/h5,10H,4,6-8H2,1
InchiKey: NKLIKTPCJUTOBJ-UHFFFAOYSA-N
Formula: C12H19ClF2O2
SMILES: CC(C)=CCCC(C)CCOC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 268.73

Physical Properties

Property code	Value	Unit	Source
gf	-513.24	kJ/mol	Joback Method
hf	-850.37	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	52.57	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.134		Crippen Method
mcvol	198.860	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1354.00		NIST Webbook
tb	586.59	K	Joback Method
tc	767.61	K	Joback Method
tf	296.64	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.27	J/mol×K	586.59	Joback Method
cpg	510.82	J/mol×K	616.76	Joback Method
cpg	524.58	J/mol×K	646.93	Joback Method
cpg	537.61	J/mol×K	677.10	Joback Method
cpg	549.92	J/mol×K	707.27	Joback Method
cpg	561.56	J/mol×K	737.44	Joback Method
cpg	572.56	J/mol×K	767.61	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=U376208&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