«beta»-Citronellol, pentafluoropropionate

Inchi: InChI=1S/C13H19F5O2/c1-9(2)5-4-6-10(3)7-8-20-11(19)12(14,15)13(16,17)18/h5,10H,4
InchiKey: QZVIRMBZIROXLA-UHFFFAOYSA-N
Formula: C13H19F5O2
SMILES: CC(C)=CCCC(C)CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 302.28

Physical Properties

Property code	Value	Unit	Source
gf	-1074.48	kJ/mol	Joback Method
hf	-1452.35	kJ/mol	Joback Method
hfus	28.15	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.500		Crippen Method
mcvol	206.020	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1336.90		NIST Webbook
tb	566.62	K	Joback Method
tc	729.39	K	Joback Method
tf	282.18	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.30	J/mol×K	566.62	Joback Method
cpg	557.15	J/mol×K	593.75	Joback Method
cpg	571.21	J/mol×K	620.88	Joback Method
cpg	584.52	J/mol×K	648.00	Joback Method
cpg	597.12	J/mol×K	675.13	Joback Method
cpg	609.03	J/mol×K	702.26	Joback Method
cpg	620.31	J/mol×K	729.39	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=U352297&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

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