Nerol, pentafluoropropionate

Inchi: InChI=1S/C13H17F5O2/c1-9(2)5-4-6-10(3)7-8-20-11(19)12(14,15)13(16,17)18/h5,7H,4,6
InchiKey: DLUDNCVSBOUXAS-YFHOEESVSA-N
Formula: C13H17F5O2
SMILES: CC(C)=CCCC(C)=CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 300.26

Physical Properties

Property code	Value	Unit	Source
gf	-1000.37	kJ/mol	Joback Method
hf	-1339.64	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	47.09	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.420		Crippen Method
mcvol	201.720	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1312.50		NIST Webbook
tb	571.10	K	Joback Method
tc	739.33	K	Joback Method
tf	278.14	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.83	J/mol×K	571.10	Joback Method
cpg	537.13	J/mol×K	599.14	Joback Method
cpg	550.61	J/mol×K	627.18	Joback Method
cpg	563.31	J/mol×K	655.22	Joback Method
cpg	575.28	J/mol×K	683.25	Joback Method
cpg	586.57	J/mol×K	711.29	Joback Method
cpg	597.22	J/mol×K	739.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352646&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