Nerol, heptafluorobutyrate

Inchi: InChI=1S/C14H17F7O2/c1-9(2)5-4-6-10(3)7-8-23-11(22)12(15,16)13(17,18)14(19,20)21/
InchiKey: NMYHVVFTLHEZBN-YFHOEESVSA-N
Formula: C14H17F7O2
SMILES: CC(C)=CCCC(C)=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 350.27

Physical Properties

Property code	Value	Unit	Source
gf	-1378.73	kJ/mol	Joback Method
hf	-1761.25	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.055		Crippen Method
mcvol	219.350	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	1383.60		NIST Webbook
tb	589.29	K	Joback Method
tc	751.85	K	Joback Method
tf	293.01	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.53	J/mol×K	589.29	Joback Method
cpg	606.80	J/mol×K	616.38	Joback Method
cpg	620.22	J/mol×K	643.48	Joback Method
cpg	632.82	J/mol×K	670.57	Joback Method
cpg	644.67	J/mol×K	697.66	Joback Method
cpg	655.81	J/mol×K	724.75	Joback Method
cpg	666.30	J/mol×K	751.85	Joback Method

Sources

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=U352644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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