«beta»-Citronellol, heptafluorobutyrate

Inchi: InChI=1S/C14H19F7O2/c1-9(2)5-4-6-10(3)7-8-23-11(22)12(15,16)13(17,18)14(19,20)21/
InchiKey: YCJAGTWYIJIPQF-UHFFFAOYSA-N
Formula: C14H19F7O2
SMILES: CC(C)=CCCC(C)CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 352.29

Physical Properties

Property code	Value	Unit	Source
gf	-1452.84	kJ/mol	Joback Method
hf	-1873.96	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	45.96	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.135		Crippen Method
mcvol	223.650	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	1363.40		NIST Webbook
tb	584.81	K	Joback Method
tc	742.55	K	Joback Method
tf	297.05	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.50	J/mol×K	584.81	Joback Method
cpg	627.34	J/mol×K	611.10	Joback Method
cpg	641.36	J/mol×K	637.39	Joback Method
cpg	654.58	J/mol×K	663.68	Joback Method
cpg	667.05	J/mol×K	689.97	Joback Method
cpg	678.82	J/mol×K	716.26	Joback Method
cpg	689.93	J/mol×K	742.55	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=U352295&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