(.+/-.)-Lavandulol, pentafluoropropionate

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

Physical Properties

Property code	Value	Unit	Source
gf	-995.19	kJ/mol	Joback Method
hf	-1336.71	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	46.07	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.276		Crippen Method
mcvol	201.720	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1269.00		NIST Webbook
tb	563.18	K	Joback Method
tc	730.73	K	Joback Method
tf	266.46	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.80	J/mol×K	563.18	Joback Method
cpg	536.34	J/mol×K	591.10	Joback Method
cpg	550.05	J/mol×K	619.03	Joback Method
cpg	562.98	J/mol×K	646.95	Joback Method
cpg	575.18	J/mol×K	674.88	Joback Method
cpg	586.68	J/mol×K	702.80	Joback Method
cpg	597.52	J/mol×K	730.73	Joback Method

Sources

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=U352631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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