(-)-Isolongifolol, pentafluoropropionate

Inchi: InChI=1S/C18H25F5O2/c1-15(2)7-4-8-16(3)11-6-5-10(13(11)15)12(16)9-25-14(24)17(19
InchiKey: LVKNWPLEJLNUEW-UHFFFAOYSA-N
Formula: C18H25F5O2
SMILES: CC1(C)CCCC2(C)C(COC(=O)C(F)(F)C(F)(F)F)C3CCC2C31
Mol. weight [g/mol]: 368.38

Physical Properties

Property code	Value	Unit	Source
gf	-977.67	kJ/mol	Joback Method
hf	-1482.16	kJ/mol	Joback Method
hfus	26.56	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.216		Crippen Method
mcvol	248.190	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1648.00		NIST Webbook
tb	692.65	K	Joback Method
tc	887.38	K	Joback Method
tf	454.43	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.75	J/mol×K	692.65	Joback Method
cpg	814.76	J/mol×K	725.11	Joback Method
cpg	833.90	J/mol×K	757.56	Joback Method
cpg	852.39	J/mol×K	790.02	Joback Method
cpg	870.45	J/mol×K	822.47	Joback Method
cpg	888.29	J/mol×K	854.93	Joback Method
cpg	906.14	J/mol×K	887.38	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=U375551&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