(-)-Isolongifolol, trifluoroacetate

Inchi: InChI=1S/C17H25F3O2/c1-15(2)7-4-8-16(3)11-6-5-10(13(11)15)12(16)9-22-14(21)17(18
InchiKey: DBEVQQPQZZVOSV-UHFFFAOYSA-N
Formula: C17H25F3O2
SMILES: CC1(C)CCCC2(C)C(COC(=O)C(F)(F)F)C3CCC2C31
Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	-599.31	kJ/mol	Joback Method
hf	-1060.55	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.581		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	674.46	K	Joback Method
tc	877.39	K	Joback Method
tf	439.56	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.11	J/mol×K	674.46	Joback Method
cpg	740.78	J/mol×K	708.28	Joback Method
cpg	760.52	J/mol×K	742.10	Joback Method
cpg	779.54	J/mol×K	775.92	Joback Method
cpg	798.09	J/mol×K	809.75	Joback Method
cpg	816.37	J/mol×K	843.57	Joback Method
cpg	834.61	J/mol×K	877.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375552&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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