(-)-Isolongifolol, heptafluorobutyrate

Inchi: InChI=1S/C19H25F7O2/c1-15(2)7-4-8-16(3)11-6-5-10(13(11)15)12(16)9-28-14(27)17(20
InchiKey: UZBXZJGGLZIZQD-UHFFFAOYSA-N
Formula: C19H25F7O2
SMILES: CC1(C)CCCC2(C)C(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)C3CCC2C31
Mol. weight [g/mol]: 418.39

Physical Properties

Property code	Value	Unit	Source
gf	-1356.03	kJ/mol	Joback Method
hf	-1903.77	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.851		Crippen Method
mcvol	265.820	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	710.84	K	Joback Method
tc	898.97	K	Joback Method
tf	469.30	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.87	J/mol×K	710.84	Joback Method
cpg	889.29	J/mol×K	742.20	Joback Method
cpg	907.93	J/mol×K	773.55	Joback Method
cpg	925.98	J/mol×K	804.91	Joback Method
cpg	943.66	J/mol×K	836.26	Joback Method
cpg	961.19	J/mol×K	867.62	Joback Method
cpg	978.78	J/mol×K	898.97	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=U375550&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