Linalool, pentafluoropropionate

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

Physical Properties

Property code	Value	Unit	Source
gf	-981.36	kJ/mol	Joback Method
hf	-1330.39	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.418		Crippen Method
mcvol	201.720	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1312.40		NIST Webbook
rinpol	1312.40		NIST Webbook
tb	560.51	K	Joback Method
tc	730.79	K	Joback Method
tf	297.84	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.71	J/mol×K	560.51	Joback Method
cpg	539.53	J/mol×K	588.89	Joback Method
cpg	553.42	J/mol×K	617.27	Joback Method
cpg	566.45	J/mol×K	645.65	Joback Method
cpg	578.67	J/mol×K	674.03	Joback Method
cpg	590.13	J/mol×K	702.41	Joback Method
cpg	600.88	J/mol×K	730.79	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=U352638&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