Linalol oxide, trifluoroacetate

Inchi: InChI=1S/C12H17F3O3/c1-5-11(4)7-6-8(17-11)10(2,3)18-9(16)12(13,14)15/h5,8H,1,6-7H
InchiKey: XRCYHUMSIDUMTJ-UHFFFAOYSA-N
Formula: C12H17F3O3
SMILES: C=CC1(C)CCC(C(C)(C)OC(=O)C(F)(F)F)O1
Mol. weight [g/mol]: 266.26

Physical Properties

Property code	Value	Unit	Source
gf	-737.44	kJ/mol	Joback Method
hf	-1092.83	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.994		Crippen Method
mcvol	183.400	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1128.00		NIST Webbook
rinpol	1128.00		NIST Webbook
tb	576.08	K	Joback Method
tc	773.45	K	Joback Method
tf	359.14	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.98	J/mol×K	576.08	Joback Method
cpg	512.60	J/mol×K	608.97	Joback Method
cpg	528.11	J/mol×K	641.87	Joback Method
cpg	542.64	J/mol×K	674.76	Joback Method
cpg	556.31	J/mol×K	707.66	Joback Method
cpg	569.23	J/mol×K	740.55	Joback Method
cpg	581.52	J/mol×K	773.45	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=U375718&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