(-)-Myrtenol, trifluoroacetate

Inchi: InChI=1S/C12H15F3O2/c1-11(2)8-4-3-7(9(11)5-8)6-17-10(16)12(13,14)15/h3,8-9H,4-6H
InchiKey: RPMAMEDCKREYSM-UHFFFAOYSA-N
Formula: C12H15F3O2
SMILES: CC1(C)C2CC=C(COC(=O)C(F)(F)F)C1C2
Mol. weight [g/mol]: 248.24

Physical Properties

Property code	Value	Unit	Source
gf	-648.82	kJ/mol	Joback Method
hf	-952.24	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	47.21	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.084		Crippen Method
mcvol	166.670	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook
tb	562.29	K	Joback Method
tc	755.59	K	Joback Method
tf	366.65	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.30	J/mol×K	562.29	Joback Method
cpg	461.89	J/mol×K	594.51	Joback Method
cpg	476.46	J/mol×K	626.72	Joback Method
cpg	490.13	J/mol×K	658.94	Joback Method
cpg	503.02	J/mol×K	691.15	Joback Method
cpg	515.24	J/mol×K	723.37	Joback Method
cpg	526.92	J/mol×K	755.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375719&Units=SI

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