Methyl pulegone

Inchi: InChI=1S/C11H18O/c1-7(2)10-6-5-8(3)9(4)11(10)12/h8-9H,5-6H2,1-4H3/t8-,9?/m0/s1
InchiKey: ZGWZVNJXOIXFSX-IENPIDJESA-N
Formula: C11H18O
SMILES: CC(C)=C1CCC(C)C(C)C1=O
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	-27.20	kJ/mol	Joback Method
hf	-307.85	kJ/mol	Joback Method
hfus	15.67	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.958		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1497.00		NIST Webbook
tb	540.30	K	Joback Method
tc	761.33	K	Joback Method
tf	281.49	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.65	J/mol×K	540.30	Joback Method
cpg	388.98	J/mol×K	577.14	Joback Method
cpg	407.37	J/mol×K	613.98	Joback Method
cpg	424.83	J/mol×K	650.81	Joback Method
cpg	441.35	J/mol×K	687.65	Joback Method
cpg	456.94	J/mol×K	724.49	Joback Method
cpg	471.58	J/mol×K	761.33	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=R440112&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

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