Methyl isopulegone

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

Physical Properties

Property code	Value	Unit	Source
gf	7.47	kJ/mol	Joback Method
hf	-278.79	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	43.55	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.814		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1464.00		NIST Webbook
tb	525.67	K	Joback Method
tc	744.10	K	Joback Method
tf	265.13	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.43	J/mol×K	525.67	Joback Method
cpg	388.69	J/mol×K	562.08	Joback Method
cpg	407.99	J/mol×K	598.48	Joback Method
cpg	426.32	J/mol×K	634.89	Joback Method
cpg	443.69	J/mol×K	671.29	Joback Method
cpg	460.08	J/mol×K	707.70	Joback Method
cpg	475.48	J/mol×K	744.10	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=R440107&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