Mint furanone I

Inchi: InChI=1S/C11H16O/c1-7-3-4-10-8(2)11(12)6-9(10)5-7/h7,9H,3-6H2,1-2H3
InchiKey: ZTLFUUKHQXBDDM-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CC1=C2CCC(C)CC2CC1=O
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	15.05	kJ/mol	Joback Method
hf	-246.11	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.712		Crippen Method
mcvol	141.400	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1291.00		NIST Webbook
tb	554.31	K	Joback Method
tc	785.16	K	Joback Method
tf	333.07	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.17	J/mol×K	554.31	Joback Method
cpg	374.07	J/mol×K	592.78	Joback Method
cpg	391.90	J/mol×K	631.26	Joback Method
cpg	408.70	J/mol×K	669.73	Joback Method
cpg	424.47	J/mol×K	708.21	Joback Method
cpg	439.25	J/mol×K	746.68	Joback Method
cpg	453.05	J/mol×K	785.16	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=R590722&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