

1-Hydroxy-2,2,6,6-tetramethyl-4-piperidinone

Inchi: InChI=1S/C9H17NO2/c1-8(2)5-7(11)6-9(3,4)10(8)12/h12H,5-6H2,1-4H3
InchiKey: KMEUSKGEUADGET-UHFFFAOYSA-N
Formula: C9H17NO2
SMILES: CC1(C)CC(=O)CC(C)(C)N1O
Mol. weight [g/mol]: 171.24
CAS: 3637-11-4

Physical Properties

Property code	Value	Unit	Source
chs	-5593.05 ± 0.42	kJ/mol	NIST Webbook
hf	-298.10 ± 4.70	kJ/mol	NIST Webbook
hfs	-378.20 ± 0.42	kJ/mol	NIST Webbook
ie	8.51 ± 0.05	eV	NIST Webbook
log10ws	-1.21		Crippen Method
logp	1.598		Crippen Method
mcvol	144.230	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	80.00	kJ/mol	308.00	NIST Webbook
hsubt	80.10 ± 4.30	kJ/mol	288.00	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3637114&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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