3-Hydroxy-2,2,4,4-tetramethylcyclobutanone, oxime

Inchi: InChI=1S/C8H15NO2/c1-7(2)5(9-11)8(3,4)6(7)10/h6,10-11H,1-4H3/b9-5-
InchiKey: JCMRJYODKOZJDF-UITAMQMPSA-N
Formula: C8H15NO2
SMILES: CC1(C)C(=NO)C(C)(C)C1O
Mol. weight [g/mol]: 157.21
CAS: 13900-80-6

Physical Properties

Property code	Value	Unit	Source
hf	-415.44	kJ/mol	Joback Method
hvap	68.07	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	1.244		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
tb	648.11	K	Joback Method
tc	842.25	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13900806&Units=SI
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

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature