«alpha»-Ketocyclododecanone oxime

Other names: 1,2-Cyclododecandione, monooxime
Inchi: InChI=1S/C12H21NO2/c14-12-10-8-6-4-2-1-3-5-7-9-11(12)13-15/h15H,1-10H2
InchiKey: DFZPTACRIAQCIW-UHFFFAOYSA-N
Formula: C12H21NO2
SMILES: O=C1CCCCCCCCCCC1=NO
Mol. weight [g/mol]: 211.30
CAS: 4422-06-4

Physical Properties

Property code	Value	Unit	Source
hf	-502.21	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
ie	8.99 ± 0.03	eV	NIST Webbook
log10ws	-2.84		Crippen Method
logp	3.300		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	762.96	K	Joback Method
tc	1005.07	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4422064&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
ie:	Ionization energy
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

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