

Cyclododecanone, oxime

Inchi: InChI=1S/C12H23NO/c14-13-12-10-8-6-4-2-1-3-5-7-9-11-12/h14H,1-11H2
InchiKey: SCRFXJBEIINMIC-UHFFFAOYSA-N
Formula: C12H23NO
SMILES: ON=C1CCCCCCCCCCC1
Mol. weight [g/mol]: 197.32
CAS: 946-89-4

Physical Properties

Property code	Value	Unit	Source
hf	-364.51	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
ie	8.84 ± 0.03	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	4.121		Crippen Method
mcvol	180.630	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	695.14	K	Joback Method
tc	926.94	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C946894&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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