2-Chlorocyclododecanone oxime

Other names: «alpha»-Chlorocyclododecanone oxime
Inchi: InChI=1S/C12H22ClNO/c13-11-9-7-5-3-1-2-4-6-8-10-12(11)14-15/h11,15H,1-10H2
InchiKey: PMQJQOIUPPQMCK-UHFFFAOYSA-N
Formula: C12H22ClNO
SMILES: ON=C1CCCCCCCCCCC1Cl
Mol. weight [g/mol]: 231.76
CAS: 4806-74-0

Physical Properties

Property code	Value	Unit	Source
hf	-400.59	kJ/mol	Joback Method
hvap	68.97	kJ/mol	Joback Method
ie	9.18 ± 0.03	eV	NIST Webbook
log10ws	-3.82		Crippen Method
logp	4.339		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	727.90	K	Joback Method
tc	962.40	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4806740&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

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