1,2-Cyclododecandione, monooxime

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]: 211.31

Physical Properties

Property code	Value	Unit	Source
hf	-368.32	kJ/mol	Cheméo Relay (1.0)
hvap	82.80	kJ/mol	Cheméo Relay (1.0)
ie	8.99 ± 0.03	eV	NIST Webbook
logp	3.300		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
tb	603.75	K	Cheméo Relay (1.0)
tf	398.96	K	Cheméo Relay (1.0)

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4422064&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point