

2-Chlorocyclooctanone, oxime

Inchi:	InChI=1S/C8H14ClNO/c9-7-5-3-1-2-4-6-8(7)10-11/h7,11H,1-6H2
InchiKey:	CLUUAPBIIZAOJL-UHFFFAOYSA-N
Formula:	C8H14ClNO
SMILES:	ON=C1CCCCCCC1Cl
Mol. weight [g/mol]:	175.66

Physical Properties

Property code	Value	Unit	Source
ie	9.19 ± 0.03	eV	NIST Webbook
logp	2.778		Crippen Method
mcvol	136.510	ml/mol	McGowan Method

Sources

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=C10499339&Units=SI
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

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/52-355-0/2-Chlorocyclooctanone-oxime.pdf>

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