

Cyclooctyne

Inchi: InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-6H2
InchiKey: ZPWOOKQUDFIEIX-UHFFFAOYSA-N
Formula: C8H12
SMILES: C1#CCCCCCC1
Mol. weight [g/mol]: 108.18
CAS: 1781-78-8

Physical Properties

Property code	Value	Unit	Source
ie	8.90	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.344		Crippen Method
mcvol	104.120	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1781788&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/41-157-2/Cyclooctyne.pdf>

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