

1,2-Cyclononadiene

Inchi:	InChI=1S/C9H14/c1-2-4-6-8-9-7-5-3-1/h1,5H,2,4,6-9H2
InchiKey:	YHGPUHUSTRYSIC-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	C1=CCCCCCCC=1
Mol. weight [g/mol]:	122.21
CAS:	1123-11-1

Physical Properties

Property code	Value	Unit	Source
ie	8.87	eV	NIST Webbook
log10ws	-3.21		Crippen Method
logp	3.052		Crippen Method
mcvol	118.210	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/13-750-4/1-2-Cyclononadiene.pdf>

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