

# 3,9-Diazaoctacyclo[9.3.22,10.0.03,9.04,8.05,15.07,1

**Other names:** 3,9-Diazaoctacyclo[9.3.2  
**Inchi:** InChI=1S/C14H18N2/c1-2-5-6(3-1)12-10-8-4-7-9(10)11(5)15-13(7)14(8)16(12)15/h5-14H  
**InchiKey:** MSQXNFZTYBJBK-UHFFFAOYSA-N  
**Formula:** C14H18N2  
**SMILES:** C1CC2C(C1)C1C3C4CC5C3C2N2C5C4N12  
**Mol. weight [g/mol]:** 214.31  
**CAS:** 70873-24-4

## Physical Properties

Property code	Value	Unit	Source
ie	7.63	eV	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.333		Crippen Method
mcvol	152.060	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C70873244&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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/61-685-4/3-9-Diazaoctacyclo-9-3-22-10-0-03-9-04-8-05-15-07-16-tetradecane.pdf>

Generated by Cheméo on 2024-05-01 19:26:00.60776638 +0000 UTC m=+16880809.528343693.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.