1,3,6,8-Tetraazatricyclo(4.4.1.1(3,8))dodecane

Other names:	1,3,6,8-tetraazatricyclo[4.4.1.1(3,8)]dodecane
	1,4,6,9-Tetraazatricyclo-(4.4.1.1
Inchi:	InChI=1S/C8H16N4/c1-2-10-7-11-3-4-12(8-10)6-9(1)5-11/h1-8H2
InchiKey:	YHNNUDUEGSHVGJ-UHFFFAOYSA-N
Formula:	C8H16N4
SMILES:	C1CN2CN3CCN(CN1C3)C2
Mol. weight [g/mol]:	168.24
CAS:	51-46-7

Physical Properties

Property code	Value	Unit	Source
ie	7.39	eV	NIST Webbook
log10ws	0.88		Crippen Method
logp	-0.935		Crippen Method
mcvol	130.920	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Osmotic and activity coefficients of two macrocyclic aminals in aqueous solution at 288.15, 293.15, 298.15 and 308.15 K:	https://www.doi.org/10.1016/j.fluid.2010.03.012
Solubility of 1,3,6,8-tetraazatricyclo[4.4.1.13,8]dodecane (TATD) in Water at Temperatures between 275 K and 303 K:	https://www.doi.org/10.1021/je700304z
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51467&Units=SI

Legend

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