1,6-Diazatetracyclo[4.3.27,9.12,5]dodecane

Other names:	1,6-Diazatetracyclo[4.3.2
Inchi:	InChI=1S/C10H16N2/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h7-10H,1-6H2
InchiKey:	YCWBYOYZBJXATQ-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	C1CC2CC1N1C3CCC(C3)N21
Mol. weight [g/mol]:	164.25
CAS:	105090-34-4

Physical Properties

Property code	Value	Unit	Source
ie	6.20 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.375		Crippen Method
mcvol	128.280	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105090344&Units=SI

Legend

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

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