

1,3,6,9b-Tetraazaphenalene

Other names: 1,3,6-Triazacycl[3.3.3]azine
Inchi: InChI=1S/C9H6N4/c1-2-7-10-5-4-9-12-6-11-8(3-1)13(7)9/h1-6H
InchiKey: MAEGTYLEMVJXMV-UHFFFAOYSA-N
Formula: C9H6N4
SMILES: C1=CC2=NC=CC3=NC=NC(=C1)N23
Mol. weight [g/mol]: 170.17
CAS: 37159-99-2

Physical Properties

Property code	Value	Unit	Source
ie	7.20	eV	NIST Webbook
ie	7.36	eV	NIST Webbook
log10ws	-1.87		Crippen Method
logp	1.066		Crippen Method
mcvol	119.210	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=C37159992&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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