

4-Chloro-6-methyl-1,3,3a,7-tetrazaindene

Inchi:	InChI=1S/C6H5ClN4/c1-4-2-5(7)11-6(10-4)8-3-9-11/h2-3H,1H3
InchiKey:	NOIPEBKPGPZXNR-UHFFFAOYSA-N
Formula:	C6H5ClN4
SMILES:	Cc1cc(Cl)n2ncnc2n1
Mol. weight [g/mol]:	168.58
CAS:	24415-66-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	1.086		Crippen Method
mcvol	108.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24415665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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