

1,5-Naphthyridine

Other names:	1,5-Diazanaphthalene 1,5-Pyridopyridine
Inchi:	InChI=1S/C8H6N2/c1-3-7-8(9-5-1)4-2-6-10-7/h1-6H
InchiKey:	VMLKTERJLVWEJJ-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1cnc2cccnc2c1
Mol. weight [g/mol]:	130.15
CAS:	254-79-5

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C254795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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