

1,8-Naphthyridine

Other names:	1,8-Diazanaphthalene 1,8-Pyridopyridine
Inchi:	InChI=1S/C8H6N2/c1-3-7-4-2-6-10-8(7)9-5-1/h1-6H
InchiKey:	FLBAYUMRQUHISI-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1cnc2ncccc2c1
Mol. weight [g/mol]:	130.15
CAS:	254-60-4

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C254604&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

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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