

1,7-Naphthyridine

Other names:	1,7-Diazanaphthalene 1,7-Pyridopyridine
Inchi:	InChI=1S/C8H6N2/c1-2-7-3-5-9-6-8(7)10-4-1/h1-6H
InchiKey:	MXBVNILGVJVMH-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1cnc2cnccc2c1
Mol. weight [g/mol]:	130.15
CAS:	253-69-0

Physical Properties

Property code	Value	Unit	Source
ie	8.99	eV	NIST Webbook
ie	8.99	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=C253690&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

Latest version available from:

<https://www.cheméo.com/cid/60-525-2/1-7-Naphthyridine.pdf>

Generated by Cheméo on 2024-04-17 03:11:35.422175632 +0000 UTC m=+15612744.342752943.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.