1H-Pyrrolo[2,3-b]pyridine

Other names:	1,7-Diazaindene
	7-Aza-1-pyrindine
	7-Azaindole
	7H-Pyrrolo[2,3-b]pyridine
	Pyrrolo(2,3-b)pyridine
	1,7-Dideazapurine
Inchi:	InChI=1S/C7H6N2/c1-2-6-3-5-9-7(6)8-4-1/h1-5H,(H,8,9)
InchiKey:	MVXVYAKCVDQRLW-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	c1cnc2[nH]ccc2c1
Mol. weight [g/mol]:	118.14
CAS:	271-63-6

Physical Properties

Property code	Value	Unit	Source
affp	940.20	kJ/mol	NIST Webbook
basg	908.30	kJ/mol	NIST Webbook
ie	8.11 ± 0.00	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	1.081		Crippen Method
mcvol	90.530	ml/mol	McGowan Method
rinpol	1292.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	220.25		NIST Webbook
rinpol	223.70		NIST Webbook
rinpol	220.25		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C271636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices