

9H-Purine

Other names:	7H-Purine 1H-Purine Purine «beta»-Purine Isopurine 3,5,7-Triazaindole 6H-Imidazo[4,5-d]pyrimidine Imidazo(4,5-d)pyrimidine NSC 753 X 128 7H-Imidazo(4,5-d)pyrimidine
Inchi:	InChI=1S/C5H4N4/c1-4-5(8-2-6-1)9-3-7-4/h1-3H,(H,6,7,8,9)
InchiKey:	KDCGOANMDULRCW-UHFFFAOYSA-N
Formula:	C5H4N4
SMILES:	<chem>c1ncc2nc[nH]c2n1</chem>
Mol. weight [g/mol]:	120.11
CAS:	120-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	-0.129		Crippen Method
mcvol	82.310	ml/mol	McGowan Method
rmpol	1474.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120730&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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