

2,6-Diaminopurine

Other names:	1H-purine-2,6-diamine 2-aminoadenine 9H-purine-2,6-diamine NSC 743 Purine, 2,6-diamino- Purine, 2,6-diamio- SQ 21065 X 79 purine-2,6-diylldiamine
Inchi:	InChI=1S/C5H6N6/c6-3-2-4(9-1-8-2)11-5(7)10-3/h1H,(H5,6,7,8,9,10,11)
InchiKey:	MSSXOMSJDRHRMC-UHFFFAOYSA-N
Formula:	C5H6N6
SMILES:	<chem>N=c1[nH]c2ncnc-2c(N)[nH]1</chem>
Mol. weight [g/mol]:	150.14
CAS:	1904-98-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	-1.665		Crippen Method
mcvol	102.270	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=C1904989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Equilibrium partitioning of drug molecules between aqueous and amino acid ester-based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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