

9H-purine, 6,9-diamino-

Inchi:	InChI=1S/C5H6N6/c6-4-3-5(9-1-8-4)11(7)2-10-3/h1-2H,7H2,(H2,6,8,9)
InchiKey:	PMYVWIREDVGFIM-UHFFFAOYSA-N
Formula:	C5H6N6
SMILES:	Nc1ncnc2c1ncn2N
Mol. weight [g/mol]:	150.14
CAS:	137062-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	-0.878		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137062874&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

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

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<https://www.chemeo.com/cid/88-078-9/9H-purine-6-9-diamino.pdf>

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