

9H-purine, 6-hydrazino-

Inchi:	InChI=1S/C5H6N6/c6-11-5-3-4(8-1-7-3)9-2-10-5/h1-2H,6H2,(H2,7,8,9,10,11)
InchiKey:	IUEISQYNCXVHTJ-UHFFFAOYSA-N
Formula:	C5H6N6
SMILES:	NNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	150.14
CAS:	5404-86-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	-0.843		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=C5404864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/88-079-8/9H-purine-6-hydrazino.pdf>

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