9H-purine, 9-cyclohex-2-enyl-6-hydrazino-

Inchi:	InChI=1S/C11H14N6/c12-16-10-9-11(14-6-13-10)17(7-15-9)8-4-2-1-3-5-8/h2,4,6-8H,1,3,
InchiKey:	PTKGJBVNKJGCPC-UHFFFAOYSA-N
Formula:	C11H14N6
SMILES:	NNc1ncnc2c1ncn2C1C=CCCC1
Mol. weight [g/mol]:	230.27
CAS:	100058-19-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	1.393		Crippen Method
mcvol	171.650	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=C100058193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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