

9H-purine, 6-hydrazino-9-(2-hydroxycyclohexyl)-, cis-

Inchi:	InChI=1S/C11H16N6O/c12-16-10-9-11(14-5-13-10)17(6-15-9)7-3-1-2-4-8(7)18/h5-8,18H
InchiKey:	ONORGJBBTBGRNG-UHFFFAOYSA-N
Formula:	C11H16N6O
SMILES:	NNc1ncnc2c1ncn2C1CCCCC1O
Mol. weight [g/mol]:	248.28
CAS:	116402-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	0.588		Crippen Method
mcvol	181.820	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402756&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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