

Hypoxanthine, 9-(2-hydroxycyclohexyl)-, trans

Inchi:	InChI=1S/C11H14N4O2/c16-8-4-2-1-3-7(8)15-6-14-9-10(15)12-5-13-11(9)17/h5-8,16H,1
InchiKey:	MRUIYTLBMWPOQV-UHFFFAOYSA-N
Formula:	C11H14N4O2
SMILES:	O=c1[nH]cnc2c1ncn2C1CCCCC1O
Mol. weight [g/mol]:	234.25
CAS:	6975-27-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	0.114		Crippen Method
mcvol	167.730	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975275&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/26-323-4/Hypoxanthine-9-2-hydroxycyclohexyl-trans.pdf>

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