

# Semicarbazide, 4-cyclohexyl-1-(4-hydroxy-6-methyl-2-pyrimidinyl) (keto form)

InChI: InChI=1S/C12H19N5OS/c1-8-7-10(18)15-11(13-8)16-17-12(19)14-9-5-3-2-4-6-9/h7,9H,2  
InChIKey: OZF5MAWJPPGLE-UHFFFAOYSA-N  
Formula: C12H19N5OS  
SMILES: Cc1cc(O)nc(NNC(S)=NC2CCCCC2)n1  
Mol. weight [g/mol]: 281.38  
CAS: 116435-06-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.026		Crippen Method
mcvol	213.140	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](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=C116435064&Units=SI>

## Legend

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

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