

Semicarbazide, 4-methyl-1-(2-pyrimidinyl)-

Inchi:	InChI=1S/C6H9N5O/c1-7-6(12)11-10-5-8-3-2-4-9-5/h2-4H,1H3,(H2,7,11,12)(H,8,9,10)
InchiKey:	WMTYQZVHQNYTHP-UHFFFAOYSA-N
Formula:	C6H9N5O
SMILES:	CNC(=O)NNc1ncccn1
Mol. weight [g/mol]:	167.17
CAS:	116659-63-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	-0.268		Crippen Method
mcvol	123.110	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659633&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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<https://www.chemeo.com/cid/59-101-4/Semicarbazide-4-methyl-1-2-pyrimidinyl.pdf>

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