

Uracil, 6-methyl-5-(piperidinomethyl)-

Inchi:	InChI=1S/C11H17N3O2/c1-8-9(10(15)13-11(16)12-8)7-14-5-3-2-4-6-14/h2-7H2,1H3,(H2
InchiKey:	WSTDDOLPOMWNCC-UHFFFAOYSA-N
Formula:	C11H17N3O2
SMILES:	Cc1nc(O)nc(O)c1CN1CCCCC1
Mol. weight [g/mol]:	223.27
CAS:	23213-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	1.182		Crippen Method
mcvol	172.910	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=C23213345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/83-800-1/Uracil-6-methyl-5-piperidinomethyl.pdf>

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