

1-methyluric acid

Inchi:	InChI=1S/C6H6N4O3/c1-10-4(11)2-3(9-6(10)13)8-5(12)7-2/h1H3,(H,9,13)(H2,7,8,12)
InchiKey:	QFDRTQONISXGJA-UHFFFAOYSA-N
Formula:	C6H6N4O3
SMILES:	Cn1c(=O)[nH]c2[nH]c(=O)[nH]c2c1=O
Mol. weight [g/mol]:	182.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	-3.203		Crippen Method
mcvol	114.010	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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