

2,4(1H,3H)-Pyrimidinedione, 6-amino-1-methyl-

Other names:	6-Amino-1-methyl-1H-pyrimidine-2,4-dione 6-Amino-1-methyluracil
Inchi:	InChI=1S/C5H7N3O2/c1-8-3(6)2-4(9)7-5(8)10/h2H,6H2,1H3,(H,7,9,10)
InchiKey:	GZLZRPNUDBIQBM-UHFFFAOYSA-N
Formula:	C5H7N3O2
SMILES:	Cn1c(N)cc(=O)[nH]c1=O
Mol. weight [g/mol]:	141.13
CAS:	2434-53-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.46		Crippen Method
logp	-1.826		Crippen Method
mcvol	99.230	ml/mol	McGowan Method

Sources

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=C2434539&Units=SI
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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