5,6-Diamino-1,3-dimethyluracil

Other names:	2,4(1H,3H)-Pyrimidinedione, 5,6-diamino-1,3-dimethyl- Uracil, 5,6-diamino-1,3-dimethyl- 4,5-Diamino-1,3-dimethyluracil 5,6-diamino-1,3-dimethylpyrimidine-2,4(1H,3H)-dione
Inchi:	InChI=1S/C6H10N4O2/c1-9-4(8)3(7)5(11)10(2)6(9)12/h7-8H2,1-2H3
InchiKey:	BGQNOPFTJROKJE-UHFFFAOYSA-N
Formula:	C6H10N4O2
SMILES:	Cn1c(N)c(N)c(=O)n(C)c1=O
Mol. weight [g/mol]:	170.17
CAS:	5440-00-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	-1.752		Crippen Method
mcvol	123.300	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5440006&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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