6-Chloro-2,4-dihydroxy-1,3-dimethylpyrimidine

Other names:	6-Chloro-1,3-dimethyluracil
	1,3-Dimethyl-4-chlorouracil
	2,4(1H,3H)-Pyrimidinedione, 6-chloro-1,3-dimethyl-
Inchi:	InChI=1S/C6H7ClN2O2/c1-8-4(7)3-5(10)9(2)6(8)11/h3H,1-2H3
InchiKey:	VATQPUHLFQHDBD-UHFFFAOYSA-N
Formula:	C6H7ClN2O2
SMILES:	Cn1c(Cl)cc(=O)n(C)c1=O
Mol. weight [g/mol]:	174.59
CAS:	6972-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	-0.263		Crippen Method
mcvol	115.580	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=C6972276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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