

Pyrimidinone, 4(3h)-, 5-amino-6-chloro

Inchi:	InChI=1S/C4H4ClN3O/c5-3-2(6)4(9)8-1-7-3/h1H,6H2,(H,7,8,9)
InchiKey:	LVMZMDMVDWIZAL-UHFFFAOYSA-N
Formula:	C4H4ClN3O
SMILES:	<chem>Nc1c(Cl)nc[nH]c1=O</chem>
Mol. weight [g/mol]:	145.55
CAS:	3137-60-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	-0.476		Crippen Method
mcvol	91.510	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3137608&Units=SI

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/119-543-7/Pyrimidinone-4-3h-5-amino-6-chloro.pdf>

Generated by Cheméo on 2024-05-06 22:51:41.793920347 +0000 UTC m=+17325150.714497660.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.