

Pyrimidine, 4,6-dichloro-5-nitro-

Other names:	4,6-Dichloro-5-nitropyrimidine 4,6-dichloro-5-nitro-pyridine
Inchi:	InChI=1S/C4HCl2N3O2/c5-3-2(9(10)11)4(6)8-1-7-3/h1H
InchiKey:	HCTISZQLTGAYOX-UHFFFAOYSA-N
Formula:	C4HCl2N3O2
SMILES:	O=[N+](O-)c1c(Cl)ncnc1Cl
Mol. weight [g/mol]:	193.98
CAS:	4316-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	1.692		Crippen Method
mcvol	105.320	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=C4316932&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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<https://www.chemeo.com/cid/115-693-5/Pyrimidine-4-6-dichloro-5-nitro.pdf>

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