

Pyrimidine, 2,4-dichloro-5-nitro-

Inchi:	InChI=1S/C4HCl2N3O2/c5-3-2(9(10)11)1-7-4(6)8-3/h1H
InchiKey:	INUSQTPGSHFGHM-UHFFFAOYSA-N
Formula:	C4HCl2N3O2
SMILES:	O=[N+](O)c1cnc(Cl)nc1Cl
Mol. weight [g/mol]:	193.98
CAS:	49845-33-2

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49845332&Units=SI
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

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/12-227-6/Pyrimidine-2-4-dichloro-5-nitro.pdf>

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