

4-Pyrimidinol, 6-chloro-5-nitro-

Inchi:	InChI=1S/C4H2ClN3O3/c5-3-2(8(10)11)4(9)7-1-6-3/h1H,(H,6,7,9)
InchiKey:	MXCCPRWUTGSJRR-UHFFFAOYSA-N
Formula:	C4H2ClN3O3
SMILES:	O=[N+](O)c1c(O)ncnc1Cl
Mol. weight [g/mol]:	175.53
CAS:	3137-56-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	0.744		Crippen Method
mcvol	98.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3137562&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

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<https://www.chemeo.com/cid/80-724-9/4-Pyrimidinol-6-chloro-5-nitro.pdf>

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