

4-Pyrimidinol, 6-methyl-5-nitro-

Inchi:	InChI=1S/C5H5N3O3/c1-3-4(8(10)11)5(9)7-2-6-3/h2H,1H3,(H,6,7,9)
InchiKey:	JCOKXNKTIIGLPD-UHFFFAOYSA-N
Formula:	C5H5N3O3
SMILES:	Cc1ncnc(O)c1[N+](=O)[O-]
Mol. weight [g/mol]:	155.11
CAS:	25624-76-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.399		Crippen Method
mcvol	100.800	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=C25624764&Units=SI

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/116-800-4/4-Pyrimidinol-6-methyl-5-nitro.pdf>

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