

4-Pyrimidinol, 6-hydrazino-5-nitro- (keto form)

Inchi:	InChI=1S/C4H5N5O3/c5-8-3-2(9(11)12)4(10)7-1-6-3/h1H,5H2,(H2,6,7,8,10)
InchiKey:	JMHQXDHUSORWFI-UHFFFAOYSA-N
Formula:	C4H5N5O3
SMILES:	NNc1nc[nH]c(=O)c1[N+](=O)[O-]
Mol. weight [g/mol]:	171.11
CAS:	3137-55-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	-1.518		Crippen Method
mcvol	106.670	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=C3137551&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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