

# [1,2,5]Oxadiazolo[3,4-d]pyrimidine, 5,7-diamino-, 1-oxide

Inchi:	InChI=1S/C4H4N6O2/c5-2-1-3(8-4(6)7-2)9-12-10(1)11/h(H4,5,6,7,8,9)
InchiKey:	QRAJKLHQNILRIW-UHFFFAOYSA-N
Formula:	C4H4N6O2
SMILES:	Nc1nc(N)c2c(no[n+]2[O-])n1
Mol. weight [g/mol]:	168.11
CAS:	16206-19-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	-1.584		Crippen Method
mcvol	99.920	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16206192&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16206192&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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