

3(2H)-Pyridazinone

Other names:	Pyridazin-3(2H)-one 3-Pyridazinone 6-Pyridazinone Pyridazine, 3-hydroxy-
Inchi:	InChI=1S/C4H4N2O/c7-4-2-1-3-5-6-4/h1-3H,(H,6,7)
InchiKey:	AAILEWXSEQLMNI-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	Oc1ccnn1
Mol. weight [g/mol]:	96.09
CAS:	504-30-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.55		Crippen Method
logp	0.182		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

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=C504303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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