

3H-pyrimidin-4-one

Inchi:	InChI=1S/C4H4N2O/c7-4-1-2-5-3-6-4/h1-3H,(H,5,6,7)
InchiKey:	DNCYBUMDUBHIJZ-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	O=c1ccnc[nH]1
Mol. weight [g/mol]:	96.09

Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Aqueous Solubility Prediction Method
logp	-0.712		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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.cheméo.com/cid/111-694-8/3H-pyrimidin-4-one.pdf>

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