

3-Methoxy-2(1H)-pyridone

Other names:	2(1H)-Pyridinone, 3-methoxy- 3-methoxy-2-pyridone
Inchi:	InChI=1S/C6H7NO2/c1-9-5-3-2-4-7-6(5)8/h2-4H,1H3,(H,7,8)
InchiKey:	LKIMDXQLHFCXQF-UHFFFAOYSA-N
Formula:	C6H7NO2
SMILES:	COc1cccnc1O
Mol. weight [g/mol]:	125.13
CAS:	20928-63-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	0.796		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C20928636&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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