

Pyrimidine, 2-methoxy-

Other names:	2-Methoxypyrimidine
Inchi:	InChI=1S/C5H6N2O/c1-8-5-6-3-2-4-7-5/h2-4H,1H3
InchiKey:	YLZYSVYZMDJYOT-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	COc1ncccc1
Mol. weight [g/mol]:	110.11
CAS:	931-63-5

Physical Properties

Property code	Value	Unit	Source
ie	9.66 ± 0.05	eV	NIST Webbook
log10ws	-1.12		Crippen Method
logp	0.485		Crippen Method
mcvol	83.380	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=C931635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/20-523-8/Pyrimidine-2-methoxy.pdf>

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