

2-Dimethylaminopyrimidine

Inchi:	InChI=1S/C6H9N3/c1-9(2)6-7-4-3-5-8-6/h3-5H,1-2H3
InchiKey:	OUMGIYIBWRLOAF-UHFFFAOYSA-N
Formula:	C6H9N3
SMILES:	CN(C)c1ncccn1
Mol. weight [g/mol]:	123.16
CAS:	5621-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	0.543		Crippen Method
mcvol	101.580	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5621023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/60-254-3/2-Dimethylaminopyrimidine.pdf>

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