

Pyrimidine, 4-(methylamino)-

Inchi:	InChI=1S/C5H7N3/c1-6-5-2-3-7-4-8-5/h2-4H,1H3,(H,6,7,8)
InchiKey:	VERCQLOBLOLF MW-UHFFFAOYSA-N
Formula:	C5H7N3
SMILES:	CN=c1ccnc[nH]1
Mol. weight [g/mol]:	109.13
CAS:	22632-10-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	-0.542		Crippen Method
mcvol	87.490	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=C22632106&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

Latest version available from:

<https://www.chemeo.com/cid/80-814-9/Pyrimidine-4-methylamino.pdf>

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