

2-Chloro-4,6-dimethylpyrimidine

Other names:	Pyrimidine, 2-chloro-4,6-dimethyl-
Inchi:	InChI=1S/C6H7ClN2/c1-4-3-5(2)9-6(7)8-4/h3H,1-2H3
InchiKey:	RZVPFDOTMFYQHR-UHFFFAOYSA-N
Formula:	C6H7ClN2
SMILES:	Cc1cc(C)nc(Cl)n1
Mol. weight [g/mol]:	142.59
CAS:	4472-44-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.747		Crippen Method
mcvol	103.840	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=C4472440&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/69-172-5/2-Chloro-4-6-dimethylpyrimidine.pdf>

Generated by Cheméo on 2024-05-01 07:05:25.266124661 +0000 UTC m=+16836374.186701976.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.