

2-Pyrimidinecarbamonitrile, 4,6-dimethyl-

Other names:	(4,6-dimethylpyrimidin-2-yl)cyanamide
Inchi:	InChI=1S/C7H8N4/c1-5-3-6(2)11-7(10-5)9-4-8/h3H,1-2H3,(H,9,10,11)
InchiKey:	IOQKVEQARXJQKM-UHFFFAOYSA-N
Formula:	C7H8N4
SMILES:	Cc1cc(C)nc(NC#N)n1
Mol. weight [g/mol]:	148.17
CAS:	55474-90-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	0.986		Crippen Method
mcvol	117.050	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=C55474903&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/28-851-6/2-Pyrimidinecarbamonitrile-4-6-dimethyl.pdf>

Generated by Cheméo on 2024-04-20 03:47:52.785667492 +0000 UTC m=+15874121.706244804.

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