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/ci990307l

Legend

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