2,6-dimethyl-4-pyrimidinamine

Inchi: InChI=1S/C6H9N3/c1-4-3-6(7)9-5(2)8-4/h3H,1-2H3,(H2,7,8,9)
InchiKey: BJJDXAFKCKSLTE-UHFFFAOYSA-N
Formula: C6H9N3
SMILES: Cc1cc(N)nc(C)n1
Mol. weight [g/mol]: 123.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Aqueous Solubility Prediction Method
logp	0.676		Crippen Method
mcvol	101.580	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

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