

2-Amino-4,6-dimethoxypyrimidine

Other names:	2-Pyrimidinamine, 4,6-dimethoxy-4,6-dimethoxypyrimidin-2-amine
Inchi:	InChI=1S/C6H9N3O2/c1-10-4-3-5(11-2)9-6(7)8-4/h3H,1-2H3,(H2,7,8,9)
InchiKey:	LVFRCHIUUKWBLR-UHFFFAOYSA-N
Formula:	C6H9N3O2
SMILES:	COc1cc(OC)nc(N)n1
Mol. weight [g/mol]:	155.15
CAS:	36315-01-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	0.076		Crippen Method
mcvol	113.320	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.85	kJ/mol	371.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36315012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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