

2-Amino-4-methylpyrimidine

Other names:	2-Pyrimidinamine, 4-methyl- 4-methyl-2-aminopyrimidine 4-methyl-2-pyrimidinamine 4-methylpyrimidin-2-ylamine 6-Methyl-2-pyrimidinamine Pyrimidine, 2-amino-4-methyl-
Inchi:	InChI=1S/C5H7N3/c1-4-2-3-7-5(6)8-4/h2-3H,1H3,(H2,6,7,8)
InchiKey:	GHCFWKFREBNSPC-UHFFFAOYSA-N
Formula:	C5H7N3
SMILES:	<chem>Cc1cc[nH]c(=N)n1</chem>
Mol. weight [g/mol]:	109.13
CAS:	108-52-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	-0.284		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1230.00	kg/m3	298.15	Energetics of aminomethylpyrimidines: An examination of the aromaticity of nitrogen heteromonocyclic derivatives

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C108521&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Energetics of aminomethylpyrimidines: <https://www.doi.org/10.1016/j.jct.2013.03.010>
**An examination of the aromaticity of
nitrogen heteromonocyclic derivatives:**

Legend

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

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