

Pyrimidine, 4-amino-

Other names:	Pyrimidine, 4-amino- 4-Pyrimidinamine 3,4-Dihydro-4-iminopyrimidine 6-Aminopyrimidine Pyrimidin-4-ylamine 4-Pyrimidineamine
Inchi:	InChI=1S/C4H5N3/c5-4-1-2-6-3-7-4/h1-3H,(H2,5,6,7)
InchiKey:	OYRRZWATULMEPF-UHFFFAOYSA-N
Formula:	C4H5N3
SMILES:	<chem>Nc1ccncn1</chem>
Mol. weight [g/mol]:	95.10

Physical Properties

Property code	Value	Unit	Source
hf	153.13	kJ/mol	Cheméo Relay (1.0)
hvap	62.65	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
logp	0.059		Crippen Method
mcvol	73.400	ml/mol	McGowan Method
tb	493.99	K	Cheméo Relay (1.0)
tf	399.30	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591548&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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