

2(1H)Pyrimidinone,4-amino-1,N-dimethyl-

Other names:	2(1H)-Pyrimidinone,1-methyl-4-(methylamino)- 1-Methyl-4-methylaminocytosine
Inchi:	InChI=1S/C6H9N3O/c1-7-5-3-4-9(2)6(10)8-5/h3-4H,1-2H3,(H,7,8,10)
InchiKey:	VBPAOWSIZPGRAK-UHFFFAOYSA-N
Formula:	C6H9N3O
SMILES:	CNc1ccn(C)c(=O)n1
Mol. weight [g/mol]:	139.16
CAS:	6220-49-1

Physical Properties

Property code	Value	Unit	Source
ie	9.30 ± 0.10	eV	NIST Webbook
ie	8.58	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	-0.178		Crippen Method
mcvol	107.450	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	122.20 ± 0.30	kJ/mol	413.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6220491&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/36-475-5/2-1H-Pyrimidinone-4-amino-1-N-dimethyl.pdf>

Generated by Cheméo on 2024-04-29 07:22:38.160788333 +0000 UTC m=+16664607.081365648.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.