

4(1H)-Pyrimidinone, 2,6-diamino-

Other names:	2,4-Diamino-6-hydroxypyrimidine 2,6-Diamino-4-hydroxypyrimidine 2,6-Diamino-4-pyrimidinol 2,6-diamino-1H-pyrimidin-4-one
Inchi:	InChI=1S/C4H6N4O/c5-2-1-3(9)8-4(6)7-2/h1H,(H5,5,6,7,8,9)
InchiKey:	SWELIMKTDYHAOY-UHFFFAOYSA-N
Formula:	C4H6N4O
SMILES:	<chem>Nc1cc(O)nc(N)n1</chem>
Mol. weight [g/mol]:	126.12
CAS:	56-06-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.18		Crippen Method
logp	-0.653		Crippen Method
mcpvol	89.250	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	147.60 ± 0.20	kJ/mol	447.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt:	Enthalpy of sublimation at a given temperature
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/51-561-2/4-1H-Pyrimidinone-2-6-diamino.pdf>

Generated by Cheméo on 2024-04-25 16:30:11.612351861 +0000 UTC m=+16351860.532929173.

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