

2-PYRIMIDINOL

Other names:	1H-pyrimidin-2-one
Inchi:	InChI=1S/C4H4N2O/c7-4-5-2-1-3-6-4/h1-3H,(H,5,6,7)
InchiKey:	VTGOHKSTWXHQJK-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	Oc1ncccn1
Mol. weight [g/mol]:	96.09

Physical Properties

Property code	Value	Unit	Source
affp	872.70	kJ/mol	NIST Webbook
basg	841.70	kJ/mol	NIST Webbook
hf	-79.01	kJ/mol	Cheméo Relay (1.0)
ie	10.06 ± 0.05	eV	NIST Webbook
logp	0.182		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C557017&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/98-320-8/2-PYRIMIDINOL.pdf>

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