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