

1-Methyl-4(1H)-pyridinone

Inchi:	InChI=1S/C6H7NO/c1-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	OYPBUQASUUMJKG-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cn1ccc(=O)cc1
Mol. weight [g/mol]:	109.13
CAS:	695-19-2

Physical Properties

Property code	Value	Unit	Source
ie	8.48 ± 0.02	eV	NIST Webbook
ie	8.20 ± 0.03	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	0.385		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	84.00 ± 3.00	kJ/mol	403.00	NIST Webbook

Sources

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=C695192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization 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

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