

4-Piperidinone, 1-methyl-

Other names:	4-Piperidone, 1-methyl- N-Methyl-4-piperidinone N-Methyl-4-piperidone 1-Methyl-4-piperidinone 1-Methyl-4-piperidione 1-Methyl-4-piperidone 1-Methylpiperidine-4-one 1-Methylpiperidone-(4) 1-Methyl-4-oxopiperidine
Inchi:	InChI=1S/C6H11NO/c1-7-4-2-6(8)3-5-7/h2-5H2,1H3
InchiKey:	HUUPVABNAQUEJW-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	CN1CCC(=O)CC1
Mol. weight [g/mol]:	113.16
CAS:	1445-73-4

Physical Properties

Property code	Value	Unit	Source
hvap	54.20 ± 1.00	kJ/mol	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	0.281		Crippen Method
mvol	96.090	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.20	K	1.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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=C1445734&Units=SI

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
t_{brp}:	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/92-371-8/4-Piperidinone-1-methyl.pdf>

Generated by Cheméo on 2024-05-03 12:05:22.461501799 +0000 UTC m=+17027171.382079110.

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