2(1H)-PYRIDINONE, 1-METHYL-

Other names:	1-Methyl-1,2-dihydro-2-pyridinone
	1-Methyl-1H-pyridin-2-one
	1-Methyl-2(1H)-pyridinone
	1-Methyl-2(1H)-pyridone
	1-Methyl-2-oxopyridine
	1-Methyl-2-pyridinone
	1-Methyl-2-pyridone
	1-methylpyridine-2-one
	2(1H)-Pyridone, 1-methyl-
	N-Methyl-2-pyridone
	N-Methylpyridone
	NSC 9383
Inchi:	InChI=1S/C6H7NO/c1-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	DVVGIUUJYPYENY-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cn1ccccc1=O
Mol. weight [g/mol]:	109.13

Physical Properties

Property code	Value	Unit	Source
affp	925.80	kJ/mol	NIST Webbook
basg	894.80	kJ/mol	NIST Webbook
hf	-73.88	kJ/mol	Cheméo Relay (1.0)
hvap	73.30	kJ/mol	Cheméo Relay (1.0)
ie	8.58 ± 0.02	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.41 ± 0.03	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
log10ws	0.96		Aqueous Solubility Prediction Method
logp	0.385		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
tb	501.63	K	Cheméo Relay (1.0)
tf	303.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.20	kJ/mol	376.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.20	K	98.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C694859&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point