

4-NITROPYRIDINE 1-OXIDE

Other names:	4-nitropyridine N-oxide 4-nitropyridine oxide 4-nitropyridine-N-oxide Avitrol 100 Pyridine-1-oxide, 4-nitro- p-nitropyridine N-oxide pyridine, 4-nitro-, 1-oxide pyridine, 4-nitro-, N-oxide
Inchi:	InChI=1S/C5H4N2O3/c8-6-3-1-5(2-4-6)7(9)10/h1-4H
InchiKey:	RXKNNAKAVAHBNK-UHFFFAOYSA-N
Formula:	C5H4N2O3
SMILES:	O=[N+](O-)c1cc[n+](O-)cc1
Mol. weight [g/mol]:	140.10

Physical Properties

Property code	Value	Unit	Source
affp	868.00	kJ/mol	NIST Webbook
basg	837.30	kJ/mol	NIST Webbook
chs	-2556.30 ± 0.50	kJ/mol	NIST Webbook
chs	-2551.00 ± 1.70	kJ/mol	NIST Webbook
hf	126.00 ± 0.90	kJ/mol	NIST Webbook
hfs	11.70 ± 1.70	kJ/mol	NIST Webbook
hfs	17.10 ± 0.80	kJ/mol	NIST Webbook
hsub	108.90 ± 0.30	kJ/mol	NIST Webbook
hsub	108.90 ± 0.30	kJ/mol	NIST Webbook
hsub	89.10 ± 2.50	kJ/mol	NIST Webbook
hvap	79.17	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-0.69		Aqueous Solubility Prediction Method
logp	0.228		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
tb	523.70	K	Cheméo Relay (1.0)
tf	433.95	K	Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	89.10 ± 2.50	kJ/mol	323.00	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):

Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation: <https://www.doi.org/10.1016/j.jct.2019.04.014>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124330&Units=SI>

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
tf:	Normal melting (fusion) point

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