Pyridine, 4-nitro-, 1-oxide

Other names:	4-Nitropyridine 1-oxide
	4-Nitropyridine N-oxide
	4-Nitropyridine oxide
	4-nitropyridine-N-oxide
	Avitrol 100
	Pyridine-1-oxide, 4-nitro-
	p-Nitropyridine 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
CAS:	1124-33-0

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	17.10 ± 0.80	kJ/mol	NIST Webbook
hfs	11.70 ± 1.70	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
log10ws	-0.69		Aqueous Solubility Prediction Method
logp	0.228		Crippen Method
mcvol	90.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hsubt	89.10 ± 2.50	kJ/mol	323.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume