

Oxiniac acid

Other names:	3-Pyridinecarboxylic acid, 1-oxide Nicotinic acid, 1-oxide Nicotinic acid oxide Nicotinic acid N-oxide Pyridine-3-carboxylic acid N-oxide 3-Carboxypyridine N-oxide 3-Pyridinecarboxylic acid oxide N-Hydroxynicotinic acid NSC 93890
Inchi:	InChI=1S/C6H5NO3/c8-6(9)5-2-1-3-7(10)4-5/h1-4H,(H,8,9)
InchiKey:	FJCFFCXMEXZEIM-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1ccc[n+][O-]c1
Mol. weight [g/mol]:	139.11
CAS:	2398-81-4

Physical Properties

Property code	Value	Unit	Source
chs	-2698.20 ± 0.70	kJ/mol	NIST Webbook
hf	-225.10 ± 2.20	kJ/mol	NIST Webbook
hfs	-377.40 ± 1.10	kJ/mol	NIST Webbook
hsub	152.30 ± 1.90	kJ/mol	NIST Webbook
hsub	152.30 ± 1.90	kJ/mol	NIST Webbook
log10ws	-3.06		Crippen Method
logp	0.018		Crippen Method
mvol	94.930	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2398814&Units=SI

Legend

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

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