

3-PYRIDINOL N-OXIDE

Other names:	3-Hydroxypyridine 1-oxide 3-hydroxypyridine-N-oxide Pyridinium,1,3-dihydroxy-,1-hydroxide,inner salt pyridin-3-ol 1-oxide
Inchi:	InChI=1S/C5H5NO2/c7-5-2-1-3-6(8)4-5/h1-4,7H
InchiKey:	YMEZKRMAPQIBQH-UHFFFAOYSA-N
Formula:	C5H5NO2
SMILES:	[O-][n+]1cccc(O)c1
Mol. weight [g/mol]:	111.10

Physical Properties

Property code	Value	Unit	Source
hf	-29.47	kJ/mol	Cheméo Relay (1.0)
hsub	121.80 ± 4.40	kJ/mol	NIST Webbook
ie	8.60 ± 0.05	eV	NIST Webbook
logp	0.026		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
tf	462.85	K	Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6602284&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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