2-PYRIDINECARBOXYLIC ACID N-OXIDE

Other names:	2-Carboxypyridine N-oxide
	2-Pyridinecarboxylic acid oxide
	2-Pyridinecarboxylic acid, 1-oxide
	Picolinic acid 1-oxide
	Pyridine-2-carboxylic acid N-oxide
	Pyridine-2-carboxylic acid, 1-oxide
	picolinic acid N-oxide
Inchi:	InChI=1S/C6H5NO3/c8-6(9)5-3-1-2-4-7(5)10/h1-4H,(H,8,9)
InchiKey:	FHYMLBVGNFVFBT-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1cccc[n+]1[O-]
Mol. weight [g/mol]:	139.11

Physical Properties

Property code	Value	Unit	Source
hf	-209.53	kJ/mol	Cheméo Relay (1.0)
hsub	94.40 ± 4.00	kJ/mol	NIST Webbook
ie	8.68	eV	Cheméo Relay (1.0)
logp	0.018		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
tf	436.95	K	Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C824408&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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