ISONICOTINONITRILE 1-OXIDE

Other names: 4-Cyanopyridine-N-oxide
Isonicotinonitrile, 1-oxide
4-Cyanopyridine oxide
4-Cyanopyridine 1-oxide
Inchi: InChI=1S/C6H4N2O/c7-5-6-1-3-8(9)4-2-6/h1-4H
InchiKey: QNCSFBSIWVBTHE-UHFFFAOYSA-N
Formula: C6H4N2O
SMILES: N#Cc1cc[n+]([O-])cc1
Mol. weight [g/mol]: 120.11

Physical Properties

Property code	Value	Unit	Source
af	0.4037		Cheméo Relay (1.0)
affp	873.40	kJ/mol	NIST Webbook
basg	842.70	kJ/mol	NIST Webbook
gf	320.44	kJ/mol	Cheméo Relay (1.0, beta)
hf	285.37	kJ/mol	Cheméo Relay (1.0)
hsub	104.40 ± 4.30	kJ/mol	NIST Webbook
hvap	73.16	kJ/mol	Cheméo Relay (1.0)
ie	8.95 ± 0.02	eV	NIST Webbook
log10ws	-0.02		Cheméo Relay (1.0)
logp	0.192		Crippen Method
mcvol	88.870	ml/mol	McGowan Method
pc	4527.18	kPa	Cheméo Relay (1.0, beta)
tb	520.46	K	Cheméo Relay (1.0)
tc	742.53	K	Cheméo Relay (1.0)
tf	483.52	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14906593&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

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point