Picolinonitrile, 1-oxide

Other names: pyridine-2-carbonitrile 1-oxide
2-Pyridinecarbonitrile, 1-oxide
Inchi: InChI=1S/C6H4N2O/c7-5-6-3-1-2-4-8(6)9/h1-4H
InchiKey: XXDJXMMIVUCDGP-UHFFFAOYSA-N
Formula: C6H4N2O
SMILES: N#Cc1cccc[n+]1[O-]
Mol. weight [g/mol]: 120.11
CAS: 2402-98-4

Physical Properties

Property code	Value	Unit	Source
ie	8.96 ± 0.02	eV	NIST Webbook
log10ws	-3.35		Crippen Method
logp	0.192		Crippen Method
mcvol	88.870	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2402984&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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