

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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<https://www.chemeo.com/cid/42-380-3/Picolinonitrile-1-oxide.pdf>

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