

Picolinic acid N-oxide

Other names:	2-Pyridinecarboxylic acid, 1-oxide Picolinic acid 1-oxide Pyridine-2-carboxylic acid N-oxide 2-Carboxypyridine N-oxide 2-Pyridinecarboxylic acid oxide Pyridine-2-carboxylic acid, 1-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+](O-)
Mol. weight [g/mol]:	139.11
CAS:	824-40-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	0.018		Crippen Method
mcvol	94.930	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=C824408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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