

Isonicotinic acid N-oxide

Other names:	4-Pyridinecarboxylic acid, 1-oxide pyridin-N-oxide-4-carboxylic acid Pyridine-4-carboxylic acid N-oxide
Inchi:	InChI=1S/C6H5NO3/c8-6(9)5-1-3-7(10)4-2-5/h1-4H,(H,8,9)
InchiKey:	QCWTWMJMLSKQCJ-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1cc[n+][O-]cc1
Mol. weight [g/mol]:	139.11
CAS:	13602-12-5

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13602125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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