

4-Pyridinecarboxaldehyde, oxime

Other names:	4-(Hydroxyiminomethyl)pyridine Isonicotinaldehyde, oxime 4-Pyridinealdoxime Pyridine-4-carboxaldoxime Pyridine-4-aldoxime 4-Pyridinecarbaldehyde oxime Pyridine, 4-formyl-, oxime NSC 63847
Inchi:	InChI=1S/C6H6N2O/c9-8-5-6-1-3-7-4-2-6/h1-5,9H
InchiKey:	OFYLBLSSPQTTHT-UHFFFAOYSA-N
Formula:	C6H6N2O
SMILES:	ON=Cc1ccncc1
Mol. weight [g/mol]:	122.12
CAS:	696-54-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	0.890		Crippen Method
mvol	93.170	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=C696548&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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