

3-Pyridineoxamic acid, ethyl ester

Inchi:	InChI=1S/C9H10N2O3/c1-2-14-9(13)8(12)11-7-4-3-5-10-6-7/h3-6H,2H2,1H3,(H,11,12)
InchiKey:	DSMSFNXXCMCOLU-UHFFFAOYSA-N
Formula:	C9H10N2O3
SMILES:	CCOC(=O)C(=O)Nc1cccnc1
Mol. weight [g/mol]:	194.19
CAS:	53117-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Crippen Method
logp	0.583		Crippen Method
mcvol	142.880	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C53117172&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/11-857-8/3-Pyridineoxamic-acid-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-20 02:31:17.33517793 +0000 UTC m=+15869526.255755245.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.