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: DSMSFNNXCMCOLU-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/ci990307l
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