

Pyridine, 4-phenoxy-, 1-oxide

Inchi:	InChI=1S/C11H9NO2/c13-12-8-6-11(7-9-12)14-10-4-2-1-3-5-10/h1-9H
InchiKey:	TYEPZEMCJSMYDJ-UHFFFAOYSA-N
Formula:	C11H9NO2
SMILES:	[O-][n+]1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	187.19
CAS:	33399-53-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	2.112		Crippen Method
mcvol	140.050	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=C33399530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/27-573-6/Pyridine-4-phenoxy-1-oxide.pdf>

Generated by Cheméo on 2024-04-26 18:00:35.562790283 +0000 UTC m=+16443684.483367599.

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