2-Phenoxynicotinic acid

Other names:	2-Phenoxypyridine-3-carboxylic acid
	3-Pyridinecarboxylic acid, 2-phenoxy-
Inchi:	InChI=1S/C12H9NO3/c14-12(15)10-7-4-8-13-11(10)16-9-5-2-1-3-6-9/h1-8H,(H,14,15)
InchiKey:	CQGAXJGXGLVFGJ-UHFFFAOYSA-N
Formula:	C12H9NO3
SMILES:	O=C(O)c1cccnc1Oc1ccccc1
Mol. weight [g/mol]:	215.20
CAS:	35620-71-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.572		Crippen Method
mcvol	155.710	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35620714&Units=SI
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

Legend

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

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