2-Phenoxypyridine-3-carbonitrile

Other names:	3-Pyridinecarbonitrile, 2-phenoxy- 2-phenoxynicotinonitrile
Inchi:	InChI=1S/C12H8N2O/c13-9-10-5-4-8-14-12(10)15-11-6-2-1-3-7-11/h1-8H
InchiKey:	KMQFYNLYTMIJPI-UHFFFAOYSA-N
Formula:	C12H8N2O
SMILES:	N#Cc1cccnc1Oc1ccccc1
Mol. weight [g/mol]:	196.20
CAS:	14178-15-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	2.746		Crippen Method
mcvol	149.650	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=C14178155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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