

3-Pyridinecarboxylic acid, 2-propenyl ester

Other names:	Nicotinic acid, allyl ester Pyridine-3-carboxylic acid, allyl ester Allyl nicotinate Nicotinic acid, prop-2-enyl ester
Inchi:	InChI=1S/C9H9NO2/c1-2-6-12-9(11)8-4-3-5-10-7-8/h2-5,7H,1,6H2
InchiKey:	SJUZXMLTUGZSSQ-UHFFFAOYSA-N
Formula:	C9H9NO2
SMILES:	<chem>C=CCOC(=O)c1cccnc1</chem>
Mol. weight [g/mol]:	163.17
CAS:	25635-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.424		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
rinpola	1278.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25635125&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/51-281-3/3-Pyridinecarboxylic-acid-2-propenyl-ester.pdf>

Generated by Cheméo on 2024-04-19 14:29:29.08641699 +0000 UTC m=+15826218.006994302.

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