

2-Quinolinecarboxylic acid, methyl ester

Other names:	Quinaldic acid, methyl ester Methyl quinaldate Methyl ester of Quinoline-2-carboxylic acid Methyl 2-quinolinecarboxylate
Inchi:	InChI=1S/C11H9NO2/c1-14-11(13)10-7-6-8-4-2-3-5-9(8)12-10/h2-7H,1H3
InchiKey:	CILJSZLWPHTUIP-UHFFFAOYSA-N
Formula:	C11H9NO2
SMILES:	<chem>COC(=O)c1ccc2ccccc2n1</chem>
Mol. weight [g/mol]:	187.19
CAS:	19575-07-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.021		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
rinpola	1711.70		NIST Webbook
rinpola	1711.70		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19575076&Units=SI

Legend

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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/40-612-7/2-Quinolinecarboxylic-acid-methyl-ester.pdf>

Generated by Cheméo on 2024-04-27 03:13:06.265510672 +0000 UTC m=+16476835.186087987.

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