

Ethyl 2-methylnicotinate

Other names:	3-Pyridinecarboxylic acid, 2-methyl-, ethyl ester
Inchi:	InChI=1S/C9H11NO2/c1-3-12-9(11)8-5-4-6-10-7(8)2/h4-6H,3H2,1-2H3
InchiKey:	TZORNSWZUZDUCU-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)c1cccnc1C
Mol. weight [g/mol]:	165.19
CAS:	1721-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.567		Crippen Method
mcvol	131.330	ml/mol	McGowan Method

Sources

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=C1721262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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