

3,5-Pyridinedicarboxylic acid, 2,4,6-trimethyl-, diethyl ester

Other names:	3,5-Diethoxycarbonyl-2,4,6-trimethylpyridine
Inchi:	InChI=1S/C14H19NO4/c1-6-18-13(16)11-8(3)12(14(17)19-7-2)10(5)15-9(11)4/h6-7H2,1-
InchiKey:	IJHKOUDBKFONBB-UHFFFAOYSA-N
Formula:	C14H19NO4
SMILES:	CCOC(=O)c1c(C)nc(C)c(C(=O)OCC)c1C
Mol. weight [g/mol]:	265.31
CAS:	1150-55-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.360		Crippen Method
mcvol	209.220	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1150556&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

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