

Diethyl pyridine-3,4-dicarboxylate

Other names:	Cinchomeric ester Diethyl 3,4-pyridinedicarboxylate Pyridine-3,4-dicarboxylic acid diethyl ester
Inchi:	InChI=1S/C11H13NO4/c1-3-15-10(13)8-5-6-12-7-9(8)11(14)16-4-2/h5-7H,3-4H2,1-2H3
InchiKey:	SIOSRDUNOOIMCE-UHFFFAOYSA-N
Formula:	C11H13NO4
SMILES:	CCOC(=O)c1ccncc1C(=O)OCC
Mol. weight [g/mol]:	223.23
CAS:	1678-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.435		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1678520&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
rinpol:	Non-polar retention indices

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