

2,6-Pyridinedicarboxylic acid, diisobutyl ester

Inchi:	InChI=1S/C15H21NO4/c1-10(2)8-19-14(17)12-6-5-7-13(16-12)15(18)20-9-11(3)4/h5-7,10
InchiKey:	UPYVVXCPRSKLAD-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]:	279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	2.707		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpola	1956.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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