

2,6-Pyridinedicarboxylic acid, butyl isopropyl ester

Inchi:	InChI=1S/C14H19NO4/c1-4-5-9-18-13(16)11-7-6-8-12(15-11)14(17)19-10(2)3/h6-8,10H,
InchiKey:	LIBLDICEOSXCLW-UHFFFAOYSA-N
Formula:	C14H19NO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OC(C)C)n1
Mol. weight [g/mol]:	265.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.604		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinsol	1894.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinsol:	Non-polar retention indices

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