2,6-Pyridinedicarboxylic acid, butyl hexyl ester

Inchi:	InChI=1S/C17H25NO4/c1-3-5-7-8-13-22-17(20)15-11-9-10-14(18-15)16(19)21-12-6-4-2/l
InchiKey:	PQZPVYCGDFLGNB-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	CCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]:	307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.776		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U368773&Units=SI

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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