

2,6-Pyridinedicarboxylic acid, isobutyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H27NO4/c1-6-8-16(13(4)5)23-18(21)15-10-7-9-14(19-15)17(20)22-11-12(2)
InchiKey:	HLXHNGNUNDKDDE-UHFFFAOYSA-N
Formula:	C18H27NO4
SMILES:	CCCC(OC(=O)c1cccc(C(=O)OCC(C)C)n1)C(C)C
Mol. weight [g/mol]:	321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	3.876		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368851&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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