

2,6-Pyridinedicarboxylic acid, isobutyl 3-methylbutyl ester

Inchi:	InChI=1S/C16H23NO4/c1-11(2)8-9-20-15(18)13-6-5-7-14(17-13)16(19)21-10-12(3)4/h5-
InchiKey:	BIAZYGJTTLVXFT-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CC(C)CCOC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]:	293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	3.097		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U368314&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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