

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

Inchi: InChI=1S/C16H23NO4/c1-5-12(4)10-21-16(19)14-8-6-7-13(17-14)15(18)20-9-11(2)3/h6-
InchiKey: MVDMAFNJJAXQJU-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCC(C)COC(=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	2063.00		NIST Webbook
rinpol	2063.00		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=U369058&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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