

2,6-Pyridinedicarboxylic acid, propyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C18H27NO4/c1-6-10-22-16(20)14-8-7-9-15(19-14)17(21)23-12-13(2)11-18(3,4)
InchiKey: NJVRBVJVODBHAF-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.877		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook

Sources

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=U368788&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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