

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

Inchi: InChI=1S/C18H27NO4/c1-5-7-12-22-17(20)14-10-8-11-15(19-14)18(21)23-16(9-6-2)13(3)
InchiKey: RJJHLVIZVIPQPT-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCOC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	4.020		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpola	2177.00		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=U369101&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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