

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

Inchi: InChI=1S/C19H29NO4/c1-6-9-14(5)23-18(21)15-11-8-12-16(20-15)19(22)24-17(10-7-2)1
InchiKey: MFOFOGFXIFUSKF-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCC(C)OC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	4.409		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpole	2175.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U368335&Units=SI>

Legend

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

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