

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

Inchi: InChI=1S/C19H29NO4/c1-6-9-17(13(3)4)24-19(22)16-11-8-10-15(20-16)18(21)23-12-14
InchiKey: ZVZDQMUTEUYRJO-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCC(OC(=O)c1cccc(C(=O)OCC(C)CC)n1)C(C)C
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	4.266		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinsol	2229.00		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=U369061&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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