

2,6-Pyridinedicarboxylic acid, di(2-methylpentyl) ester

Inchi: InChI=1S/C19H29NO4/c1-5-8-14(3)12-23-18(21)16-10-7-11-17(20-16)19(22)24-13-15(4)
InchiKey: CSJACVWNPZUZQI-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCC(C)COC(=O)c1cccc(C(=O)OCC(C)CCC)n1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.268		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpola	2336.00		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=U369099&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
rinpola: Non-polar retention indices

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