

2,6-Pyridinedicarboxylic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C23H37NO4/c1-16(12-22(3,4)5)14-27-20(25)18-10-9-11-19(24-18)21(26)28-15
InchiKey: CJIGHZBOSRMTMZ-UHFFFAOYSA-N
Formula: C23H37NO4
SMILES: CC(COC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1)CC(C)(C)C
Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	5.540		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpole	2529.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368805&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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