

2,6-Pyridinedicarboxylic acid, isobutyl tridecyl ester

Inchi: InChI=1S/C24H39NO4/c1-4-5-6-7-8-9-10-11-12-13-14-18-28-23(26)21-16-15-17-22(25-2
InchiKey: FNMSQNLRHWRSJX-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	6.362		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		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=U368859&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
rinpol: Non-polar retention indices

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