

2,6-Pyridinedicarboxylic acid, 5-methoxy-3-methylpent-2-yl undecyl ester

Inchi: InChI=1S/C25H41NO5/c1-5-6-7-8-9-10-11-12-13-18-30-24(27)22-15-14-16-23(26-22)25
InchiKey: BOBQFBJNGUFICP-UHFFFAOYSA-N
Formula: C25H41NO5
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1
Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	5.987		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
rinpol	2989.00		NIST Webbook
rinpol	2989.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369177&Units=SI>
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>

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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