

2,6-Pyridinedicarboxylic acid, 3-methylbutyl tridecyl ester

Inchi: InChI=1S/C25H41NO4/c1-4-5-6-7-8-9-10-11-12-13-14-19-29-24(27)22-16-15-17-23(26-2
InchiKey: LMYXAQQGTAVMIA-UHFFFAOYSA-N
Formula: C25H41NO4
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.18		Crippen Method
logp	6.752		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
rinpol	2987.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368325&Units=SI>

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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