

2,6-Pyridinedicarboxylic acid, pentadecyl pentyl ester

Inchi: InChI=1S/C27H45NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-23-32-27(30)25-21-19-20
InchiKey: VCJKHOIFIKMELL-UHFFFAOYSA-N
Formula: C27H45NO4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.26		Crippen Method
logp	7.677		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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=U368293&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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