

2,6-Pyridinedicarboxylic acid, isopropyl octadecyl ester

Inchi: InChI=1S/C28H47NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-32-27(30)25-2
InchiKey: XVLQDKKPJAHEIR-UHFFFAOYSA-N
Formula: C28H47NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C)n1
Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.79		Crippen Method
logp	8.065		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinsol	3190.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U369163&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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