

Isonicotinic acid, 4-tridecyl ester

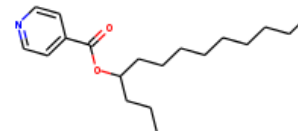
InChI: InChI=1S/C19H31NO2/c1-3-5-6-7-8-9-10-12-18(11-4-2)22-19(21)17-13-15-20-16-14-17/h13-16,18H,3-12H2,1-2H3

InChI Key: VOKUCSCZSOGBRE-UHFFFAOYSA-N

Formula: C19H31NO2

SMILES: CCCCCCCCC(CCC)OC(=O)c1ccncc1

Molecular Weight: 305.45



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	5.55		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H31NO2/c1-3-5-6-7-8-9-10-12-18\(11-4-2\)22-19\(21\)17-13-15-20-16-14-17/h13-16,18H,3-12H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H31NO2/c1-3-5-6-7-8-9-10-12-18(11-4-2)22-19(21)17-13-15-20-16-14-17/h13-16,18H,3-12H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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