

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/
InchiKey: VOKUCSCZSOGBRE-UHFFFAOYSA-N
Formula: C19H31NO2
SMILES: CCCCCCCCC(CCC)OC(=O)c1cncc1
Mol. weight [g/mol]: 305.45

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.61 | | Crippen Method |
| logp | 5.548 | | Crippen Method |
| mcvol | 272.230 | ml/mol | McGowan Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U299895&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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