

Isonicoinic acid, 5-tridecyl ester

Inchi: InChI=1S/C19H31NO2/c1-3-5-7-8-9-10-12-18(11-6-4-2)22-19(21)17-13-15-20-16-14-17/
InchiKey: DVXIBZJEHOPKSW-UHFFFAOYSA-N
Formula: C19H31NO2
SMILES: CCCCCCCCC(CCCC)OC(=O)c1ccncc1
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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299896&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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