

Isonicotinic acid, 3-tetradecyl ester

Inchi: InChI=1S/C20H33NO2/c1-3-5-6-7-8-9-10-11-12-13-19(4-2)23-20(22)18-14-16-21-17-15-
InchiKey: GSUPFAAVLAQWJM-UHFFFAOYSA-N
Formula: C20H33NO2
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1ccncc1
Mol. weight [g/mol]: 319.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.938		Crippen Method
mcvol	286.320	ml/mol	McGowan Method

Sources

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=U299898&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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