Isonicotinic acid, hexadecyl ester

Inchi: InChI=1S/C22H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-25-22(24)21-16-18-23-
InchiKey: STUBJXFCGLTLMA-UHFFFAOYSA-N
Formula: C22H37NO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 347.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	6.720		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
rinpol	2617.00		NIST Webbook

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=U299891&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
rinpol: Non-polar retention indices