Isonicotinic acid, octyl ester

Inchi: InChI=1S/C14H21NO2/c1-2-3-4-5-6-7-12-17-14(16)13-8-10-15-11-9-13/h8-11H,2-7,12H2
InchiKey: GGLVNUJXRYCZHW-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.599		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299884&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.