Isonicotinic acid, pentyl ester

Inchi: InChI=1S/C11H15NO2/c1-2-3-4-9-14-11(13)10-5-7-12-8-6-10/h5-8H,2-4,9H2,1H3
InchiKey: MZHSESFNXADKBC-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	2.429		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
rinpol	1474.00		NIST Webbook
rinpol	1474.00		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=U299881&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

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