Isonicotinic acid, cyclopentyl ester

Inchi: InChI=1S/C11H13NO2/c13-11(9-5-7-12-8-6-9)14-10-3-1-2-4-10/h5-8,10H,1-4H2
InchiKey: QPUNDERDSYMSEX-UHFFFAOYSA-N
Formula: C11H13NO2
SMILES: O=C(OC1CCCC1)c1ccncc1
Mol. weight [g/mol]: 191.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.181		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308359&Units=SI
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

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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