

Isonicotinic acid, 2,2-dimethylpropyl ester

Inchi: InChI=1S/C11H15NO2/c1-11(2,3)8-14-10(13)9-4-6-12-7-5-9/h4-7H,8H2,1-3H3
InchiKey: AYJICZOOGKSEPV-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CC(C)(C)COC(=O)c1ccncc1
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.284		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
rinpol	1363.00		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=U308335&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

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