

Isonicotinic acid, propyl ester

Inchi: InChI=1S/C9H11NO2/c1-2-7-12-9(11)8-3-5-10-6-4-8/h3-6H,2,7H2,1H3
InchiKey: TZAAGDYITBGHOB-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	1.648		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
rinpol	1271.00		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=U308345&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

Latest version available from:

<https://www.chemeo.com/cid/58-684-9/Isonicotinic-acid-propyl-ester.pdf>

Generated by Cheméo on 2025-12-05 23:53:19.916682635 +0000 UTC m=+4726997.446723289.

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