Isonipecotic acid, n-methoxycarbonyl-, propyl ester

Inchi: InChI=1S/C11H19NO4/c1-3-8-16-10(13)9-4-6-12(7-5-9)11(14)15-2/h9H,3-8H2,1-2H3
InchiKey: KJBBKJFLIWGYMY-UHFFFAOYSA-N
Formula: C11H19NO4
SMILES: CCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]: 229.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Cheméo Relay (1.0)
logp	1.418		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
rinpol	1703.00		NIST Webbook
tb	574.13	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322017&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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