Isonipecotic acid, n-propoxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H23NO4/c1-3-9-17-12(15)11-5-7-14(8-6-11)13(16)18-10-4-2/h11H,3-10H2

InchiKey: OTNHPXTUVKKALK-UHFFFAOYSA-N

Formula: C13H23NO4

SMILES: CCCOC(=O)C1CCN(C(=O)OCCC)CC1

Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	2.198		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322075&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

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