Isonipecotic acid, N-ethoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C15H27NO4/c1-4-19-15(18)16-9-7-13(8-10-16)14(17)20-11-5-6-12(2)3/h12-13

InchiKey: KZWDHPVWMDROBU-UHFFFAOYSA-N

Formula: C15H27NO4

SMILES: CCOC(=O)N1CCC(C(=O)OCCCC(C)C)CC1

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	2.834		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322005&Units=SI

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

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