Isonipecotic acid, N-isobutoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C27H51NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-31-26(29)25-18-20-2

InchiKey: GGKVMCLPMNYRCU-UHFFFAOYSA-N

Formula: C27H51NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1

Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.81		Crippen Method
logp	7.516		Crippen Method
mcvol	405.290	ml/mol	McGowan Method

Sources

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=U322074&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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