

Isonipecotic acid, N-isobutoxycarbonyl-, decyl ester

Inchi: InChI=1S/C21H39NO4/c1-4-5-6-7-8-9-10-11-16-25-20(23)19-12-14-22(15-13-19)21(24)2
InchiKey: QEEUQDXJFAKUKS-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	5.175		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rmpol	2624.00		NIST Webbook
rmpol	2624.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322069&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rmpol: Non-polar retention indices

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