

Isonipecotic acid, n-butoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C22H41NO4/c1-3-5-7-8-9-10-11-12-13-19-26-21(24)20-14-16-23(17-15-20)22
InchiKey: MPSDLNDWIVSWQV-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.709		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
rinpole	2791.00		NIST Webbook
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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=U322056&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
rinpole: Non-polar retention indices

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