

Isonipecotic acid, n-butoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-23-30-25(28)24-18-20-27
InchiKey: OJWSGJXQJWWKAL-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	7.269		Crippen Method
mcvol	391.200	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322059&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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