

Pipecolic acid, N-hexyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C24H45NO4/c1-3-5-7-9-10-11-12-13-17-20-28-23(26)22-18-14-15-19-25(22)24
InchiKey: WUAVDIQJFHKSJI-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCCC
Mol. weight [g/mol]: 411.62

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.15 | | Crippen Method |
| logp | 6.632 | | Crippen Method |
| mcvol | 363.020 | ml/mol | McGowan Method |
| rinpol | 2899.00 | | NIST Webbook |
| rinpol | 2899.00 | | NIST Webbook |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393116&Units=SI>

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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