

Isonipecotic acid, N-(cyclohexylcarbonyl)-, tridecyl ester

Inchi: InChI=1S/C26H47NO3/c1-2-3-4-5-6-7-8-9-10-11-15-22-30-26(29)24-18-20-27(21-19-24)
InchiKey: PXZPGSCPIKBVME-UHFFFAOYSA-N
Formula: C26H47NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 421.66

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.22 | | Crippen Method |
| logp | 6.659 | | Crippen Method |
| mcvol | 374.470 | ml/mol | McGowan Method |
| rinpola | 3386.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361036&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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