

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

Inchi: InChI=1S/C16H27NO3/c1-2-12-20-16(19)14-8-10-17(11-9-14)15(18)13-6-4-3-5-7-13/h13-15,17-19,20
InchiKey: JRXJGMSXIMOFJC-UHFFFAOYSA-N
Formula: C16H27NO3
SMILES: CCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 281.39

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.03 | | Crippen Method |
| logp | 2.758 | | Crippen Method |
| mcvol | 233.570 | ml/mol | McGowan Method |
| rinpola | 2320.00 | | NIST Webbook |
| rinpola | 2320.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361025&Units=SI>

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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