

Isonipecotic acid, N-(3-phenylpropionyl)-, hexyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C21H31NO3/c1-2-3-4-8-17-25-21(24)19-13-15-22(16-14-19)20(23)12-11-18-9 |
| InchiKey: | KQCOKBNSQGDGCF-UHFFFAOYSA-N |
| Formula: | C21H31NO3 |
| SMILES: | CCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1 |
| Mol. weight [g/mol]: | 345.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.58 | | Crippen Method |
| logp | 3.981 | | Crippen Method |
| mcvol | 291.120 | ml/mol | McGowan Method |
| rinpol | 2892.00 | | 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=U361559&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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