

Isonipecotic acid, N-(4-nitrobenzoyl)-, propyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C16H20N2O5/c1-2-11-23-16(20)13-7-9-17(10-8-13)15(19)12-3-5-14(6-4-12)18 |
| InchiKey: | LMGWLHCMDIYSDF-UHFFFAOYSA-N |
| Formula: | C16H20N2O5 |
| SMILES: | CCCOC(=O)C1CCN(C(=O)c2ccc([N+](=O)[O-])cc2)CC1 |
| Mol. weight [g/mol]: | 320.34 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.71 | | Crippen Method |
| logp | 2.400 | | Crippen Method |
| mcvol | 238.090 | ml/mol | McGowan Method |
| rinpol | 2798.00 | | 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=U361041&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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