

# Isonipecotic acid, N-(4-butylbenzoyl)-, heptyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C24H37NO3/c1-3-5-7-8-9-19-28-24(27)22-15-17-25(18-16-22)23(26)21-13-11 |
| InchiKey:            | XINFYBYFDULBGC-UHFFFAOYSA-N   |
| Formula:             | C24H37NO3   |
| SMILES:              | CCCCCCCOC(=O)C1CCN(C(=O)c2ccc(CCCC)cc2)CC1                                      |
| Mol. weight [g/mol]: | 387.56  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.38   |        | Crippen Method |
| logp          | 5.395   |        | Crippen Method |
| mcvol         | 333.390 | ml/mol | McGowan Method |
| rinpol        | 3216.00 |        | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361134&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361134&amp;Units=SI</a> |

## 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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