

# Butyl 3-furylpropanoate

|                      |                                                                            |
|----------------------|----------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H16O3/c1-2-3-7-14-11(12)5-4-10-6-8-13-9-10/h6,8-9H,2-5,7H2,1H3 |
| InchiKey:            | GKBPVNJYWGTECJ-UHFFFAOYSA-N                                                |
| Formula:             | C11H16O3                                                                   |
| SMILES:              | CCCCOC(=O)CCc1ccoc1                                                        |
| Mol. weight [g/mol]: | 196.24                                                                     |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.96   |        | Crippen Method |
| logp          | 2.555   |        | Crippen Method |
| mcvol         | 159.700 | ml/mol | McGowan Method |
| rinpol        | 1354.00 |        | NIST Webbook   |
| rinpol        | 1354.00 |        | NIST Webbook   |
| ripol         | 1728.00 |        | NIST Webbook   |
| ripol         | 1728.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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=R508000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R508000&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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         |
| ripol:   | Polar retention indices             |

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