

# Terephthalic acid, but-2-enyl tridecyl ester

**Inchi:** InChI=1S/C25H38O4/c1-3-5-7-8-9-10-11-12-13-14-15-21-29-25(27)23-18-16-22(17-19-20)24  
**InchiKey:** CAPLXHPCMGAEI-GQCTYLIASA-N  
**Formula:** C25H38O4  
**SMILES:** CC=CCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCC)cc1  
**Mol. weight [g/mol]:** 402.57

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -125.22 | kJ/mol  | Joback Method  |
| hf            | -706.65 | kJ/mol  | Joback Method  |
| hfus          | 59.93   | kJ/mol  | Joback Method  |
| hvap          | 92.45   | kJ/mol  | Joback Method  |
| log10ws       | -8.09   |         | Crippen Method |
| logp          | 6.887   |         | Crippen Method |
| mcvol         | 349.930 | ml/mol  | McGowan Method |
| pc            | 1002.71 | kPa     | Joback Method  |
| rinpol        | 3110.00 |         | NIST Webbook   |
| tb            | 959.80  | K       | Joback Method  |
| tc            | 1175.26 | K       | Joback Method  |
| tf            | 549.69  | K       | Joback Method  |
| vc            | 1.355   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1153.14   | J/mol×K | 959.80          | Joback Method |
| cpg           | 1170.06   | J/mol×K | 995.71          | Joback Method |
| cpg           | 1185.67   | J/mol×K | 1031.62         | Joback Method |
| cpg           | 1200.03   | J/mol×K | 1067.53         | Joback Method |
| cpg           | 1213.20   | J/mol×K | 1103.44         | Joback Method |
| cpg           | 1225.23   | J/mol×K | 1139.35         | Joback Method |
| cpg           | 1236.18   | J/mol×K | 1175.26         | Joback Method |
| dvisc         | 0.0003167 | Pa×s    | 549.69          | Joback Method |
| dvisc         | 0.0001611 | Pa×s    | 618.04          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000938 | Pa×s | 686.39 | Joback Method |
| dvisc | 0.0000602 | Pa×s | 754.74 | Joback Method |
| dvisc | 0.0000416 | Pa×s | 823.10 | Joback Method |
| dvisc | 0.0000304 | Pa×s | 891.45 | Joback Method |
| dvisc | 0.0000233 | Pa×s | 959.80 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356321&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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