

# Phthalic acid, ethyl 2-methylpent-3-yl ester

Inchi:

LnChI=1S/C16H22O4/c1-5-14(11(3)4)20-16(18)13-10-8-7-9-12(13)15(17)19-6-2/h7-11,14

InchiKey:

UYVFSZGWMORNQD-UHFFFAOYSA-N

Formula:

C16H22O4

SMILES:

CCOC(=O)c1ccccc1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]:

278.34

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -286.10 | kJ/mol  | Joback Method  |
| hf            | -648.67 | kJ/mol  | Joback Method  |
| hfus          | 29.38   | kJ/mol  | Joback Method  |
| hvap          | 71.68   | kJ/mol  | Joback Method  |
| log10ws       | -4.34   |         | Crippen Method |
| logp          | 3.455   |         | Crippen Method |
| mcvol         | 227.420 | ml/mol  | McGowan Method |
| pc            | 1841.99 | kPa     | Joback Method  |
| rinpol        | 1879.00 |         | NIST Webbook   |
| tb            | 748.84  | K       | Joback Method  |
| tc            | 956.66  | K       | Joback Method  |
| tf            | 423.34  | K       | Joback Method  |
| vc            | 0.860   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 649.54    | J/mol×K | 748.84          | Joback Method |
| cpg           | 717.14    | J/mol×K | 922.02          | Joback Method |
| cpg           | 705.67    | J/mol×K | 887.39          | Joback Method |
| cpg           | 693.19    | J/mol×K | 852.75          | Joback Method |
| cpg           | 679.68    | J/mol×K | 818.11          | Joback Method |
| cpg           | 665.13    | J/mol×K | 783.48          | Joback Method |
| cpg           | 727.62    | J/mol×K | 956.66          | Joback Method |
| dvisc         | 0.0000793 | Pa×s    | 748.84          | Joback Method |
| dvisc         | 0.0001042 | Pa×s    | 694.59          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001432 | Pa×s | 640.34 | Joback Method |
| dvisc | 0.0002089 | Pa×s | 586.09 | Joback Method |
| dvisc | 0.0003291 | Pa×s | 531.84 | Joback Method |
| dvisc | 0.0005749 | Pa×s | 477.59 | Joback Method |
| dvisc | 0.0011585 | Pa×s | 423.34 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                     |
| <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=U356905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356905&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>                                 |

## 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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