

# Phthalic acid, 3-ethylphenyl pentyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H24O4/c1-3-5-8-14-24-20(22)18-12-6-7-13-19(18)21(23)25-17-11-9-10-16 |
| <b>InchiKey:</b>            | XXWKYUJCQBKRJF-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C21H24O4   |
| <b>SMILES:</b>              | CCCCCOC(=O)c1cccc1C(=O)Oc1cccc(CC)c1   |
| <b>Mol. weight [g/mol]:</b> | 340.41   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -136.34 | kJ/mol  | Joback Method  |
| hf            | -516.25 | kJ/mol  | Joback Method  |
| hfus          | 43.02   | kJ/mol  | Joback Method  |
| hvap          | 86.53   | kJ/mol  | Joback Method  |
| log10ws       | -6.28   |         | Crippen Method |
| logp          | 4.815   |         | Crippen Method |
| mcvol         | 274.110 | ml/mol  | McGowan Method |
| pc            | 1587.28 | kPa     | Joback Method  |
| rinpol        | 2539.00 |         | NIST Webbook   |
| tb            | 895.78  | K       | Joback Method  |
| tc            | 1118.92 | K       | Joback Method  |
| tf            | 548.63  | K       | Joback Method  |
| vc            | 1.044   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 838.22    | J/molxK | 895.78          | Joback Method |
| cpg           | 852.39    | J/molxK | 932.97          | Joback Method |
| cpg           | 865.25    | J/molxK | 970.16          | Joback Method |
| cpg           | 876.83    | J/molxK | 1007.35         | Joback Method |
| cpg           | 887.18    | J/molxK | 1044.54         | Joback Method |
| cpg           | 896.32    | J/molxK | 1081.73         | Joback Method |
| cpg           | 904.28    | J/molxK | 1118.92         | Joback Method |
| dvisc         | 0.0004108 | Paxs    | 548.63          | Joback Method |
| dvisc         | 0.0002443 | Paxs    | 606.49          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001591 | Paxs | 664.35 | Joback Method |
| dvisc | 0.0001109 | Paxs | 722.20 | Joback Method |
| dvisc | 0.0000816 | Paxs | 780.06 | Joback Method |
| dvisc | 0.0000626 | Paxs | 837.92 | Joback Method |
| dvisc | 0.0000498 | Paxs | 895.78 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357079&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357079&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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