

# Pimelic acid, hexyl octyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H40O4/c1-3-5-7-9-10-15-19-25-21(23)17-13-11-12-16-20(22)24-18-14-8-6 |
| <b>InchiKey:</b>            | BRKYWMKTVCIDRT-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C21H40O4   |
| <b>SMILES:</b>              | CCCCCCCCOC(=O)CCCCC(=O)OCCCCC  |
| <b>Mol. weight [g/mol]:</b> | 356.54   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -341.90 | kJ/mol               | Joback Method  |
| hf            | -966.37 | kJ/mol               | Joback Method  |
| hfus          | 55.72   | kJ/mol               | Joback Method  |
| hvap          | 80.65   | kJ/mol               | Joback Method  |
| log10ws       | -6.34   |                      | Crippen Method |
| logp          | 5.964   |                      | Crippen Method |
| mvol          | 321.630 | ml/mol               | McGowan Method |
| pc            | 1012.95 | kPa                  | Joback Method  |
| rinpol        | 2468.00 |                      | NIST Webbook   |
| rinpol        | 2468.00 |                      | NIST Webbook   |
| tb            | 832.46  | K                    | Joback Method  |
| tc            | 1019.85 | K                    | Joback Method  |
| tf            | 470.75  | K                    | Joback Method  |
| vc            | 1.260   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1030.26   | J/molxK | 832.46          | Joback Method |
| cpg           | 1048.96   | J/molxK | 863.69          | Joback Method |
| cpg           | 1066.54   | J/molxK | 894.92          | Joback Method |
| cpg           | 1083.03   | J/molxK | 926.15          | Joback Method |
| cpg           | 1098.44   | J/molxK | 957.39          | Joback Method |
| cpg           | 1112.80   | J/molxK | 988.62          | Joback Method |
| cpg           | 1126.13   | J/molxK | 1019.85         | Joback Method |
| dvisc         | 0.0007511 | Paxs    | 470.75          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003622 | Paxs | 531.03 | Joback Method |
| dvisc | 0.0002027 | Paxs | 591.32 | Joback Method |
| dvisc | 0.0001263 | Paxs | 651.61 | Joback Method |
| dvisc | 0.0000852 | Paxs | 711.89 | Joback Method |
| dvisc | 0.0000612 | Paxs | 772.17 | Joback Method |
| dvisc | 0.0000461 | Paxs | 832.46 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393872&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>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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