

# Malonic acid, hexyl 3-hexyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C15H28O4/c1-4-7-8-9-11-18-14(16)12-15(17)19-13(6-3)10-5-2/h13H,4-12H2,1 |
| <b>InchiKey:</b>            | TYWNYUUCYPBQQF-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H28O4   |
| <b>SMILES:</b>              | CCCCCOC(=O)CC(=O)OC(CC)CCC   |
| <b>Mol. weight [g/mol]:</b> | 272.38   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -394.86 | kJ/mol               | Joback Method  |
| hf            | -847.81 | kJ/mol               | Joback Method  |
| hfus          | 36.66   | kJ/mol               | Joback Method  |
| hvap          | 66.91   | kJ/mol               | Joback Method  |
| log10ws       | -3.94   |                      | Crippen Method |
| logp          | 3.622   |                      | Crippen Method |
| mcvol         | 237.090 | ml/mol               | McGowan Method |
| pc            | 1528.27 | kPa                  | Joback Method  |
| rinpol        | 1748.00 |                      | NIST Webbook   |
| rinpol        | 1748.00 |                      | NIST Webbook   |
| tb            | 694.74  | K                    | Joback Method  |
| tc            | 872.74  | K                    | Joback Method  |
| tf            | 388.13  | K                    | Joback Method  |
| vc            | 0.917   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 677.76    | J/molxK | 694.74          | Joback Method |
| cpg           | 751.59    | J/molxK | 843.08          | Joback Method |
| cpg           | 738.39    | J/molxK | 813.41          | Joback Method |
| cpg           | 724.41    | J/molxK | 783.74          | Joback Method |
| cpg           | 709.65    | J/molxK | 754.07          | Joback Method |
| cpg           | 694.10    | J/molxK | 724.41          | Joback Method |
| cpg           | 764.02    | J/molxK | 872.74          | Joback Method |
| dvisc         | 0.0000977 | Paxs    | 694.74          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001300 | Paxs | 643.64 | Joback Method |
| dvisc | 0.0001817 | Paxs | 592.54 | Joback Method |
| dvisc | 0.0002704 | Paxs | 541.43 | Joback Method |
| dvisc | 0.0004373 | Paxs | 490.33 | Joback Method |
| dvisc | 0.0007909 | Paxs | 439.23 | Joback Method |
| dvisc | 0.0016719 | Paxs | 388.13 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349122&amp;Units=SI</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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