

# Dodecanoic acid, 10-methyl-, methyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Methyl 10-methyldodecanoate   |
| <b>Inchi:</b>               | InChI=1S/C14H28O2/c1-4-13(2)11-9-7-5-6-8-10-12-14(15)16-3/h13H,4-12H2,1-3H3 |
| <b>InchiKey:</b>            | TXYNNTTGOJGLDCB-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C14H28O2  |
| <b>SMILES:</b>              | CCC(C)CCCCCCCC(=O)OC  |
| <b>Mol. weight [g/mol]:</b> | 228.37  |
| <b>CAS:</b>                 | 5129-65-7   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -169.36 | kJ/mol               | Joback Method  |
| hf            | -582.37 | kJ/mol               | Joback Method  |
| hfus          | 31.28   | kJ/mol               | Joback Method  |
| hvap          | 55.53   | kJ/mol               | Joback Method  |
| log10ws       | -4.30   |                      | Crippen Method |
| logp          | 4.326   |                      | Crippen Method |
| mcvol         | 215.560 | ml/mol               | McGowan Method |
| pc            | 1589.81 | kPa                  | Joback Method  |
| tb            | 595.57  | K                    | Joback Method  |
| tc            | 766.26  | K                    | Joback Method  |
| tf            | 304.70  | K                    | Joback Method  |
| vc            | 0.838   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 567.35    | J/mol×K | 595.57          | Joback Method |
| cpg           | 646.34    | J/mol×K | 737.81          | Joback Method |
| cpg           | 631.92    | J/mol×K | 709.36          | Joback Method |
| cpg           | 616.82    | J/mol×K | 680.91          | Joback Method |
| cpg           | 601.04    | J/mol×K | 652.47          | Joback Method |
| cpg           | 584.55    | J/mol×K | 624.02          | Joback Method |
| cpg           | 660.10    | J/mol×K | 766.26          | Joback Method |
| dvisc         | 0.0001432 | Paxs    | 595.57          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001938 | Paxs | 547.09 | Joback Method |
| dvisc | 0.0002782 | Paxs | 498.61 | Joback Method |
| dvisc | 0.0004318 | Paxs | 450.13 | Joback Method |
| dvisc | 0.0007451 | Paxs | 401.66 | Joback Method |
| dvisc | 0.0014934 | Paxs | 353.18 | Joback Method |
| dvisc | 0.0037349 | Paxs | 304.70 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C5129657&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129657&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>                           |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b> | Log <sub>10</sub> 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>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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