

# «alpha»-Terpinyl acetate

|                      |                                                                                                                                                                                                                                                                                                                                                      |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 3-Cyclohexene-1-methanol, «alpha»,«alpha»,4-trimethyl-, acetate<br>p-Menth-1-en-8-ol, acetate<br>«alpha»-Terpineol acetate<br>Terpinyl acetate<br>«alpha»-Terpenyl acetate<br>Terpenyl acetate<br>«alpha»-Terpinenyl acetate<br>Terpineol acetate<br>terpinenyl acetate<br>Alpha-Terpenyl acetate<br>4-Terpinyl acetate<br>p-menth-1-en-8-yl acetate |
| Inchi:               | InChI=1S/C12H20O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h5,11H,6-8H2,1-4H3/t11-/m1                                                                                                                                                                                                                                                                     |
| InchiKey:            | IGODOXYLBBOXFDW-LLVKDONJSA-N                                                                                                                                                                                                                                                                                                                         |
| Formula:             | C12H20O2                                                                                                                                                                                                                                                                                                                                             |
| SMILES:              | CC(=O)OC(C)(C)C1CC=C(C)CC1                                                                                                                                                                                                                                                                                                                           |
| Mol. weight [g/mol]: | 196.29                                                                                                                                                                                                                                                                                                                                               |
| CAS:                 | 80-26-2                                                                                                                                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -136.14 | kJ/mol | Joback Method  |
| hf            | -443.93 | kJ/mol | Joback Method  |
| hfus          | 14.88   | kJ/mol | Joback Method  |
| hvap          | 51.55   | kJ/mol | Joback Method  |
| log10ws       | -3.33   |        | Crippen Method |
| logp          | 3.075   |        | Crippen Method |
| mcvol         | 172.220 | ml/mol | McGowan Method |
| pc            | 2313.61 | kPa    | Joback Method  |
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| tc    | 785.17  | K                    | Joback Method |
| tf    | 320.24  | K                    | Joback Method |
| vc    | 0.639   | m <sup>3</sup> /kmol | Joback Method |

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| cpg           | 456.93    | J/mol×K | 606.45          | Joback Method |
| cpg           | 474.66    | J/mol×K | 642.20          | Joback Method |
| cpg           | 491.30    | J/mol×K | 677.94          | Joback Method |
| cpg           | 506.89    | J/mol×K | 713.68          | Joback Method |
| cpg           | 521.47    | J/mol×K | 749.42          | Joback Method |
| cpg           | 535.06    | J/mol×K | 785.17          | Joback Method |
| dvisc         | 0.0029306 | Pa×s    | 320.24          | Joback Method |
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| dvisc         | 0.0007919 | Pa×s    | 403.73          | Joback Method |
| dvisc         | 0.0004947 | Pa×s    | 445.48          | Joback Method |
| dvisc         | 0.0003350 | Pa×s    | 487.22          | Joback Method |
| dvisc         | 0.0002413 | Pa×s    | 528.97          | Joback Method |
| dvisc         | 0.0001823 | Pa×s    | 570.71          | Joback Method |
| hvapt         | 68.10     | kJ/mol  | 367.00          | NIST Webbook  |

## Sources

|                        |                                                                                                                                         |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C80262&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C80262&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>                       |
| <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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>ripol:</b>   | 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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