

# Bornyl acetate

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|-----------------------------|--|
| <b>Other names:</b>         | Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, endo-Borneol, acetate<br>Bornyl acetic ether<br>2-Camphanol acetate<br>endo-2-Camphanyl ethanoate<br>1,7,7-Trimethylbicyclo(2.2.1)heptan-2-ol acetate<br>borneyl acetate<br>bornyl aceate<br>1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl acetate<br>endo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate |
| <b>Inchi:</b>               | InChI=1S/C12H20O2/c1-8(13)14-10-7-9-5-6-12(10,4)11(9,2)3/h9-10H,5-7H2,1-4H3/t9?,1  |
| <b>InchiKey:</b>            | KGEKLUUHTZCSIP-YZRBQDESA-N   |
| <b>Formula:</b>             | C12H20O2   |
| <b>SMILES:</b>              | CC(=O)OC1CC2CCC1(C)C2(C)C  |
| <b>Mol. weight [g/mol]:</b> | 196.29   |
| <b>CAS:</b>                 | 76-49-3  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -100.76 | kJ/mol | Joback Method  |
| hf            | -406.57 | kJ/mol | Joback Method  |
| hfus          | 13.34   | kJ/mol | Joback Method  |
| hvap          | 48.54   | kJ/mol | Joback Method  |
| log10ws       | -2.88   |        | Crippen Method |
| logp          | 2.764   |        | Crippen Method |
| mcvol         | 165.660 | ml/mol | McGowan Method |
| pc            | 2462.92 | kPa    | Joback Method  |
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| tf    | 368.84        | K                    | Joback Method |
| vc    | 0.631         | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 521.34 | J/mol×K | 738.88          | Joback Method |
| cpg           | 437.90 | J/mol×K | 559.14          | Joback Method |
| cpg           | 456.54 | J/mol×K | 595.09          | Joback Method |
| cpg           | 474.00 | J/mol×K | 631.03          | Joback Method |
| cpg           | 490.47 | J/mol×K | 666.98          | Joback Method |
| cpg           | 506.18 | J/mol×K | 702.93          | Joback Method |
| cpg           | 536.18 | J/mol×K | 774.82          | Joback Method |
| hvapt         | 50.80  | kJ/mol  | 407.50          | NIST Webbook  |

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<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C76493&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>hvp:</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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