

# Methyl 8,11,13-Abietadien-18-oate

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H30O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2) |
| <b>InchiKey:</b>            | PGZCJOPTDHWYES-JBACZVJFSA-N  |
| <b>Formula:</b>             | C21H30O2   |
| <b>SMILES:</b>              | COC(=O)C1(C)CCCC2(C)c3ccc(C(C)C)cc3CCC12   |
| <b>Mol. weight [g/mol]:</b> | 314.46   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 61.34   | kJ/mol               | Joback Method  |
| hf            | -369.84 | kJ/mol               | Joback Method  |
| hfus          | 23.22   | kJ/mol               | Joback Method  |
| hvap          | 72.27   | kJ/mol               | Joback Method  |
| log10ws       | -5.45   |                      | Crippen Method |
| logp          | 4.993   |                      | Crippen Method |
| mcvol         | 268.710 | ml/mol               | McGowan Method |
| pc            | 1584.75 | kPa                  | Joback Method  |
| rinpol        | 2288.00 |                      | NIST Webbook   |
| tb            | 810.20  | K                    | Joback Method  |
| tc            | 1044.45 | K                    | Joback Method  |
| tf            | 507.45  | K                    | Joback Method  |
| vc            | 1.014   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 856.31 | J/mol×K | 810.20          | Joback Method |
| cpg           | 879.62 | J/mol×K | 849.24          | Joback Method |
| cpg           | 902.74 | J/mol×K | 888.28          | Joback Method |
| cpg           | 925.96 | J/mol×K | 927.33          | Joback Method |
| cpg           | 949.61 | J/mol×K | 966.37          | Joback Method |
| cpg           | 973.97 | J/mol×K | 1005.41         | Joback Method |
| cpg           | 999.36 | J/mol×K | 1044.45         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R20437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R20437&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>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>mccvol:</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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