

# 24(28)-Dihydroobtusifoliol acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C32H54O2/c1-20(2)21(3)10-11-22(4)25-14-18-32(9)28-13-12-26-23(5)29(34-2

AEUXNTWFROSOOS-AYUWEKAFSA-N

C32H54O2

CC(=O)OC1CCC2(C)C3=C(CCC2C1C)C1(C)CCC(C(C)CCC(C)C(C)C)C1(C)CC3

470.77

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 130.92  | kJ/mol  | Joback Method  |
| hf            | -684.51 | kJ/mol  | Joback Method  |
| hfus          | 37.66   | kJ/mol  | Joback Method  |
| hvap          | 92.57   | kJ/mol  | Joback Method  |
| log10ws       | -9.45   |         | Crippen Method |
| logp          | 8.986   |         | Crippen Method |
| mcvol         | 421.440 | ml/mol  | McGowan Method |
| pc            | 801.15  | kPa     | Joback Method  |
| rinpol        | 3336.00 |         | NIST Webbook   |
| rinpol        | 3336.00 |         | NIST Webbook   |
| tb            | 1050.67 | K       | Joback Method  |
| tc            | 1289.34 | K       | Joback Method  |
| tf            | 616.50  | K       | Joback Method  |
| vc            | 1.599   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1665.41 | J/mol×K | 1050.67         | Joback Method |
| cpg           | 1709.67 | J/mol×K | 1090.45         | Joback Method |
| cpg           | 1756.37 | J/mol×K | 1130.23         | Joback Method |
| cpg           | 1806.02 | J/mol×K | 1170.01         | Joback Method |
| cpg           | 1859.12 | J/mol×K | 1209.79         | Joback Method |
| cpg           | 1916.15 | J/mol×K | 1249.56         | Joback Method |
| cpg           | 1977.62 | J/mol×K | 1289.34         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R110188&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110188&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rlnpol:</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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