

# 7-Hydroxyfarnesen

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2,6,10-trimethyldodeca-2,7,9,11-tetraen-6-ol                                      |
| <b>Inchi:</b>               | InChI=1S/C15H24O/c1-6-14(4)10-8-12-15(5,16)11-7-9-13(2)3/h6,8-10,12,16H,1,7,11H2, |
| <b>InchiKey:</b>            | VJBVZYOKPWWGLN-HBMMGNRNSA-N   |
| <b>Formula:</b>             | C15H24O   |
| <b>SMILES:</b>              | <chem>C=CC(C)=CC=CC(C)(O)CCC=C(C)C</chem>   |
| <b>Mol. weight [g/mol]:</b> | 220.35  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 252.84  | kJ/mol               | Joback Method  |
| hf            | -56.40  | kJ/mol               | Joback Method  |
| hfus          | 27.99   | kJ/mol               | Joback Method  |
| hvap          | 63.73   | kJ/mol               | Joback Method  |
| log10ws       | -4.89   |                      | Crippen Method |
| logp          | 4.172   |                      | Crippen Method |
| mcvol         | 210.880 | ml/mol               | McGowan Method |
| pc            | 1827.85 | kPa                  | Joback Method  |
| ripol         | 2294.00 |                      | NIST Webbook   |
| ripol         | 2273.00 |                      | NIST Webbook   |
| tb            | 640.47  | K                    | Joback Method  |
| tc            | 828.10  | K                    | Joback Method  |
| tf            | 277.13  | K                    | Joback Method  |
| vc            | 0.806   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 554.13 | J/mol×K | 640.47          | Joback Method |
| cpg           | 569.45 | J/mol×K | 671.74          | Joback Method |
| cpg           | 583.91 | J/mol×K | 703.01          | Joback Method |
| cpg           | 597.58 | J/mol×K | 734.29          | Joback Method |
| cpg           | 610.54 | J/mol×K | 765.56          | Joback Method |
| cpg           | 622.86 | J/mol×K | 796.83          | Joback Method |
| cpg           | 634.61 | J/mol×K | 828.10          | 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=U374204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374204&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>ri pol:</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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