

# (E)-«beta»-Farnesene

|                      |                                                                                                                                                                                                                                                                                                                                                                      |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (E)-<br>7,11-Dimethyl-3-methylene-1,6,10-dodecatriene, trans<br>«beta»-Farnesene (E)<br>«beta»-trans-Farnesene<br>Farnesene (E, «beta»)<br>t-«beta»-Farnesene<br>trans-«beta»-Farnesene<br>(E)-«beta»-Farnesene<br>beta-(E)-Farnesene<br>trans-«beta»-farnesen<br>(E)-7,11-dimethyl-3-methylenedodeca-1,6,10-triene |
| Inchi:               | InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,9,12H,1,4,7-8,10-11H2,2-3,5                                                                                                                                                                                                                                                                                  |
| InchiKey:            | JSNRRGGBADWTMC-NTCAYCPXSA-N                                                                                                                                                                                                                                                                                                                                          |
| Formula:             | C15H24                                                                                                                                                                                                                                                                                                                                                               |
| SMILES:              | C=CC(=C)CCC=C(C)CCC=C(C)C                                                                                                                                                                                                                                                                                                                                            |
| Mol. weight [g/mol]: | 204.35                                                                                                                                                                                                                                                                                                                                                               |
| CAS:                 | 18794-84-8                                                                                                                                                                                                                                                                                                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | 385.89  | kJ/mol | Joback Method  |
| hf            | 103.00  | kJ/mol | Joback Method  |
| hfus          | 28.52   | kJ/mol | Joback Method  |
| hvap          | 72.50   | kJ/mol | NIST Webbook   |
| log10ws       | -5.52   |        | Crippen Method |
| logp          | 5.202   |        | Crippen Method |
| mcvol         | 205.010 | ml/mol | McGowan Method |
| pc            | 1659.19 | kPa    | Joback Method  |
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| tb    | 543.92  | K       | Joback Method |
| tc    | 730.22  | K       | Joback Method |
| tf    | 203.25  | K       | Joback Method |
| vc    | 0.800   | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 481.95 | J/mol×K | 543.92          | Joback Method |
| cpg           | 499.95 | J/mol×K | 574.97          | Joback Method |
| cpg           | 517.00 | J/mol×K | 606.02          | Joback Method |
| cpg           | 533.16 | J/mol×K | 637.07          | Joback Method |
| cpg           | 548.48 | J/mol×K | 668.12          | Joback Method |
| cpg           | 563.01 | J/mol×K | 699.17          | Joback Method |
| cpg           | 576.82 | J/mol×K | 730.22          | 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=C18794848&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18794848&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>                             |

# 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>rinpola:</b> | Non-polar retention indices                     |
| <b>ripola:</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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