

# «gamma»-Humulene

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C15H24/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h7,10,12H,2,5-6,8-9,11H2,1 |
| <b>InchiKey:</b>            | FNXUOGPQAOCFKU-PVYBRLDNSA-N  |
| <b>Formula:</b>             | C15H24   |
| <b>SMILES:</b>              | C=C1C=CC(C)(C)CCCC(C)=CCC1   |
| <b>Mol. weight [g/mol]:</b> | 204.35   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 137.25  | kJ/mol  | Joback Method  |
| hf            | -125.84 | kJ/mol  | Joback Method  |
| hfus          | 10.54   | kJ/mol  | Joback Method  |
| hvap          | 50.53   | kJ/mol  | Joback Method  |
| log10ws       | -5.32   |         | Crippen Method |
| logp          | 5.035   |         | Crippen Method |
| mcvol         | 198.450 | ml/mol  | McGowan Method |
| pc            | 2053.03 | kPa     | Joback Method  |
| rinpol        | 1483.00 |         | NIST Webbook   |
| rinpol        | 1487.00 |         | NIST Webbook   |
| rinpol        | 1483.00 |         | NIST Webbook   |
| rinpol        | 1487.00 |         | NIST Webbook   |
| ripol         | 1682.00 |         | NIST Webbook   |
| ripol         | 1682.00 |         | NIST Webbook   |
| tb            | 586.20  | K       | Joback Method  |
| tc            | 821.65  | K       | Joback Method  |
| tf            | 300.21  | K       | Joback Method  |
| vc            | 0.723   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 499.47 | J/molxK | 586.20          | Joback Method |
| cpg           | 523.64 | J/molxK | 625.44          | Joback Method |
| cpg           | 546.38 | J/molxK | 664.68          | Joback Method |
| cpg           | 567.79 | J/molxK | 703.92          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 587.97 | J/mol×K | 743.17 | Joback Method |
| cpg | 607.03 | J/mol×K | 782.41 | Joback Method |
| cpg | 625.07 | J/mol×K | 821.65 | 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=R631091&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R631091&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>mvol:</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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