

# 2-epi-(E)- «beta»-Caryophyllene

**Inchi:** InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h6,13-14H,2,5,7-10H2,1,  
**InchiKey:** NPNUFJAVOOONJE-IZZDOVSWSA-N  
**Formula:** C15H24  
**SMILES:** C=C1CCC=C(C)CCC2C1CC2(C)C  
**Mol. weight [g/mol]:** 204.35

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 14.82   | kJ/mol | Joback Method      |
| hvap          | 61.73   | kJ/mol | Cheméo Relay (1.0) |
| logp          | 4.725   |        | Crippen Method     |
| mcvol         | 191.890 | ml/mol | McGowan Method     |
| rinpol        | 1465.00 |        | NIST Webbook       |
| rinpol        | 1465.00 |        | NIST Webbook       |
| ripol         | 1669.00 |        | NIST Webbook       |
| tb            | 544.66  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 501.77 | J/mol×K | 576.30          | Joback Method |
| cpg           | 525.28 | J/mol×K | 613.93          | Joback Method |
| cpg           | 547.37 | J/mol×K | 651.55          | Joback Method |
| cpg           | 568.18 | J/mol×K | 689.18          | Joback Method |
| cpg           | 587.84 | J/mol×K | 726.81          | Joback Method |
| cpg           | 606.51 | J/mol×K | 764.43          | Joback Method |
| cpg           | 624.31 | J/mol×K | 802.06          | Joback Method |

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

|                                  |                                                                                                                                           |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>                         |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                           |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                           |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R425455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R425455&amp;Units=SI</a> |

## Legend

|                |                                                 |
|----------------|-------------------------------------------------|
| <b>cpg:</b>    | Ideal gas heat capacity                         |
| <b>hfus:</b>   | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>   | Enthalpy of vaporization at standard conditions |
| <b>logp:</b>   | Octanol/Water partition coefficient             |
| <b>mcvol:</b>  | McGowan's characteristic volume                 |
| <b>rinpol:</b> | Non-polar retention indices                     |
| <b>ripol:</b>  | Polar retention indices                         |
| <b>tb:</b>     | Normal Boiling Point Temperature                |

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