

# diepi-«alpha»-Cedrene epoxide

**Inchi:** InChI=1S/C15H24O/c1-9-5-6-10-13(2,3)11-7-15(9,10)8-12-14(11,4)16-12/h9-12H,5-8H2,  
**InchiKey:** HZRFVTRTTXBHSE-FXQPYSQLSA-N  
**Formula:** C15H24O  
**SMILES:** CC1CCC2C(C)(C)C3CC12CC1OC13C  
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 192.70  | kJ/mol  | Joback Method  |
| hf            | -209.03 | kJ/mol  | Joback Method  |
| hfus          | 19.44   | kJ/mol  | Joback Method  |
| hvap          | 48.77   | kJ/mol  | Joback Method  |
| log10ws       | -3.78   |         | Crippen Method |
| logp          | 3.626   |         | Crippen Method |
| mcvol         | 184.640 | ml/mol  | McGowan Method |
| pc            | 2244.00 | kPa     | Joback Method  |
| rinpol        | 1617.00 |         | NIST Webbook   |
| rinpol        | 1631.00 |         | NIST Webbook   |
| tb            | 583.22  | K       | Joback Method  |
| tc            | 812.69  | K       | Joback Method  |
| tf            | 416.12  | K       | Joback Method  |
| vc            | 0.716   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 540.98 | J/mol×K | 583.22          | Joback Method |
| cpg           | 563.50 | J/mol×K | 621.46          | Joback Method |
| cpg           | 584.43 | J/mol×K | 659.71          | Joback Method |
| cpg           | 604.21 | J/mol×K | 697.95          | Joback Method |
| cpg           | 623.32 | J/mol×K | 736.20          | Joback Method |
| cpg           | 642.20 | J/mol×K | 774.44          | Joback Method |
| cpg           | 661.33 | J/mol×K | 812.69          | 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=R574057&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R574057&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>hvac:</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>rinpol:</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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