

# 4,7-Epoxi-spirovetiva-2,11-diene

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | 4,7-epoxy-spirovetiva-2,11-diene                                                   |
| Inchi:               | InChI=1S/C15H22O/c1-11(2)15-9-8-14(10-15)12(3)6-5-7-13(14,4)16-15/h5,7,12H,1,6,8-1 |
| InchiKey:            | RJDKCAMBNKUPIB-LJISPDSOSA-N                                                        |
| Formula:             | C15H22O                                                                            |
| SMILES:              | C=C(C)C12CCC3(C1)C(C)CC=CC3(C)O2                                                   |
| Mol. weight [g/mol]: | 218.33                                                                             |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 232.42  | kJ/mol  | Joback Method  |
| hf            | -80.05  | kJ/mol  | Joback Method  |
| hfus          | 13.60   | kJ/mol  | Joback Method  |
| hvap          | 49.52   | kJ/mol  | Joback Method  |
| log10ws       | -4.32   |         | Crippen Method |
| logp          | 3.857   |         | Crippen Method |
| mcvol         | 186.900 | ml/mol  | McGowan Method |
| pc            | 2398.22 | kPa     | Joback Method  |
| rinpol        | 1478.00 |         | NIST Webbook   |
| tb            | 590.08  | K       | Joback Method  |
| tc            | 830.63  | K       | Joback Method  |
| tf            | 384.66  | K       | Joback Method  |
| vc            | 0.713   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 514.13 | J/mol×K | 590.08          | Joback Method |
| cpg           | 535.34 | J/mol×K | 630.17          | Joback Method |
| cpg           | 555.05 | J/mol×K | 670.26          | Joback Method |
| cpg           | 573.73 | J/mol×K | 710.36          | Joback Method |
| cpg           | 591.90 | J/mol×K | 750.45          | Joback Method |
| cpg           | 610.06 | J/mol×K | 790.54          | Joback Method |
| cpg           | 628.69 | J/mol×K | 830.63          | 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=R198762&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R198762&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>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>rinsol:</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                                 |

Latest version available from:

<https://www.cheméo.com/cid/43-497-3/4-7-Epoxy-spirovetiva-2-11-diene.pdf>

Generated by Cheméo on 2025-12-25 01:11:20.972695246 +0000 UTC m=+6373278.502735901.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.