

# 7-epi-helifolen-15-al

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C15H22O/c1-11-4-5-12-14(3,10-16)13(2)6-8-15(11,12)9-7-13/h6,8,10-12H,4-5 |
| <b>InchiKey:</b>            | IVGPPCYQIKEJMO-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C15H22O   |
| <b>SMILES:</b>              | CC1CCC2C13C=CC(C)(CC3)C2(C)C=O  |
| <b>Mol. weight [g/mol]:</b> | 218.33  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 132.02  | kJ/mol  | Joback Method  |
| hf            | -169.61 | kJ/mol  | Joback Method  |
| hfus          | 11.57   | kJ/mol  | Joback Method  |
| hvap          | 52.01   | kJ/mol  | Joback Method  |
| log10ws       | -3.71   |         | Crippen Method |
| logp          | 3.594   |         | Crippen Method |
| mcvol         | 186.900 | ml/mol  | McGowan Method |
| pc            | 2405.28 | kPa     | Joback Method  |
| rinpol        | 1591.00 |         | NIST Webbook   |
| rinpol        | 1591.00 |         | NIST Webbook   |
| tb            | 610.56  | K       | Joback Method  |
| tc            | 846.37  | K       | Joback Method  |
| tf            | 411.57  | K       | Joback Method  |
| vc            | 0.726   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 528.43 | J/molxK | 610.56          | Joback Method |
| cpg           | 549.02 | J/molxK | 649.86          | Joback Method |
| cpg           | 568.38 | J/molxK | 689.16          | Joback Method |
| cpg           | 586.96 | J/molxK | 728.46          | Joback Method |
| cpg           | 605.21 | J/molxK | 767.77          | Joback Method |
| cpg           | 623.58 | J/molxK | 807.07          | Joback Method |
| cpg           | 642.54 | J/molxK | 846.37          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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=R233568&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233568&amp;Units=SI</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>hvp:</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>rinp:</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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