

# trans-«alpha»-Phellandrene epoxide

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H16O/c1-7(2)8-4-5-10(3)9(6-8)11-10/h4-5,7-9H,6H2,1-3H3/t8-,9+,10-/m1/s |
| <b>InchiKey:</b>            | YYOYQZIEGSUHQG-KXUCPTDWSA-N  |
| <b>Formula:</b>             | C10H16O  |
| <b>SMILES:</b>              | CC(C)C1C=CC2(C)OC2C1   |
| <b>Mol. weight [g/mol]:</b> | 152.23   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 70.92   | kJ/mol               | Joback Method  |
| hf            | -194.89 | kJ/mol               | Joback Method  |
| hfus          | 16.28   | kJ/mol               | Joback Method  |
| hvap          | 40.81   | kJ/mol               | Joback Method  |
| log10ws       | -2.48   |                      | Crippen Method |
| logp          | 2.376   |                      | Crippen Method |
| mcvol         | 131.610 | ml/mol               | McGowan Method |
| pc            | 2934.52 | kPa                  | Joback Method  |
| rinsol        | 1215.00 |                      | NIST Webbook   |
| tb            | 467.19  | K                    | Joback Method  |
| tc            | 679.13  | K                    | Joback Method  |
| tf            | 266.81  | K                    | Joback Method  |
| vc            | 0.499   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 305.50 | J/mol×K | 467.19          | Joback Method |
| cpg           | 323.65 | J/mol×K | 502.51          | Joback Method |
| cpg           | 340.42 | J/mol×K | 537.84          | Joback Method |
| cpg           | 355.96 | J/mol×K | 573.16          | Joback Method |
| cpg           | 370.40 | J/mol×K | 608.48          | Joback Method |
| cpg           | 383.90 | J/mol×K | 643.81          | Joback Method |
| cpg           | 396.59 | J/mol×K | 679.13          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=R195456&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R195456&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>                                 |

# 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>mccvol:</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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