

# 7-epi-Silphiperfol-5-ene

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H24/c1-10-5-8-15-12(3)11(2)9-14(15,4)7-6-13(10)15/h9-10,12-13H,5-8H2, |
| InchiKey:            | OVRIZVNVMIWWMN-UHFFFAOYSA-N                                                       |
| Formula:             | C15H24                                                                            |
| SMILES:              | CC1=CC2(C)CCC3C(C)CCC32C1C                                                        |
| Mol. weight [g/mol]: | 204.35                                                                            |
| CAS:                 | 138752-23-5                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 227.40  | kJ/mol  | Joback Method  |
| hf            | -110.74 | kJ/mol  | Joback Method  |
| hfus          | 15.19   | kJ/mol  | Joback Method  |
| hvap          | 47.10   | kJ/mol  | Joback Method  |
| log10ws       | -4.43   |         | Crippen Method |
| logp          | 4.415   |         | Crippen Method |
| mcvol         | 185.330 | ml/mol  | McGowan Method |
| pc            | 2117.78 | kPa     | Joback Method  |
| rinpol        | 1348.00 |         | NIST Webbook   |
| rinpol        | 1348.00 |         | NIST Webbook   |
| rinpol        | 1348.00 |         | NIST Webbook   |
| rinpol        | 1348.30 |         | NIST Webbook   |
| tb            | 566.64  | K       | Joback Method  |
| tc            | 792.17  | K       | Joback Method  |
| tf            | 358.19  | K       | Joback Method  |
| vc            | 0.711   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 503.55 | J/mol×K | 566.64          | Joback Method |
| cpg           | 526.55 | J/mol×K | 604.23          | Joback Method |
| cpg           | 547.97 | J/mol×K | 641.82          | Joback Method |
| cpg           | 568.10 | J/mol×K | 679.41          | Joback Method |
| cpg           | 587.25 | J/mol×K | 716.99          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 605.70 | J/mol×K | 754.58 | Joback Method |
| cpg | 623.74 | J/mol×K | 792.17 | Joback Method |

## Sources

|                        |                                                                                                                                                 |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C138752235&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C138752235&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.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>                           |

## 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>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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