

# Helmintogermacrene

Inchi:

lnchl=1S/C15H24/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h6,9,15H,1,5,7-8,10-11H2,2

InchiKey:

XMRKUJJDDKYUHV-SOMPWSNVSA-N

Formula:

C15H24

SMILES:

C=C(C)C1CC=C(C)CCC=C(C)CC1

Mol. weight [g/mol]:

204.35

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 171.42  | kJ/mol  | Joback Method  |
| hf            | -114.99 | kJ/mol  | Joback Method  |
| hfus          | 17.12   | kJ/mol  | Joback Method  |
| hvap          | 51.42   | kJ/mol  | Joback Method  |
| log10ws       | -5.32   |         | Crippen Method |
| logp          | 5.035   |         | Crippen Method |
| mcvol         | 198.450 | ml/mol  | McGowan Method |
| pc            | 1950.95 | kPa     | Joback Method  |
| rinpol        | 1512.00 |         | NIST Webbook   |
| rinpol        | 1512.00 |         | NIST Webbook   |
| tb            | 584.07  | K       | Joback Method  |
| tc            | 810.41  | K       | Joback Method  |
| tf            | 262.95  | K       | Joback Method  |
| vc            | 0.731   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 499.67 | J/mol×K | 584.07          | Joback Method |
| cpg           | 523.53 | J/mol×K | 621.79          | Joback Method |
| cpg           | 546.01 | J/mol×K | 659.52          | Joback Method |
| cpg           | 567.11 | J/mol×K | 697.24          | Joback Method |
| cpg           | 586.84 | J/mol×K | 734.97          | Joback Method |
| cpg           | 605.21 | J/mol×K | 772.69          | Joback Method |
| cpg           | 622.25 | J/mol×K | 810.41          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R617580&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R617580&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rlnpol:</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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