

# germacrene A

**Inchi:** InChI=1S/C14H22/c1-12(2)14-9-7-5-4-6-8-13(3)10-11-14/h5,7-8,14H,1,4,6,9-11H2,2-3H3  
**InchiKey:** XNNFTAIJLZPUAI-HNVHAEGFSA-N  
**Formula:** C14H22  
**SMILES:** C=C(C)[C@@H]1C/C=C/CC/C=C(\C)CC1  
**Mol. weight [g/mol]:** 190.33

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 14.92   | kJ/mol | Joback Method      |
| hvap          | 62.86   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.45    | eV     | Cheméo Relay (1.0) |
| log10ws       | -5.18   |        | Cheméo Relay (1.0) |
| logp          | 4.645   |        | Crippen Method     |
| mcvol         | 184.360 | ml/mol | McGowan Method     |
| rinpol        | 1484.00 |        | NIST Webbook       |
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| ripol | 1743.00 |   | NIST Webbook       |
| ripol | 1700.00 |   | NIST Webbook       |
| ripol | 1747.00 |   | NIST Webbook       |
| tb    | 539.67  | K | Cheméo Relay (1.0) |
| tf    | 240.87  | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 446.33 | J/mol×K | 556.21          | Joback Method |
| cpg           | 470.16 | J/mol×K | 594.48          | Joback Method |
| cpg           | 492.58 | J/mol×K | 632.76          | Joback Method |
| cpg           | 513.60 | J/mol×K | 671.03          | Joback Method |
| cpg           | 533.26 | J/mol×K | 709.31          | Joback Method |
| cpg           | 551.56 | J/mol×K | 747.58          | Joback Method |
| cpg           | 568.51 | J/mol×K | 785.86          | Joback Method |

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C28387442&Units=SI>

|                        |                                                                                                                       |
|------------------------|-----------------------------------------------------------------------------------------------------------------------|
| <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>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>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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