

# Aromadendra-4,9-diene

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | 1,1,4,7-Tetramethyl-1a,2,4a,5,6,7b-hexahydro-1H-cyclopropa[e]azulene              |
| Inchi:               | InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h6,11-12,14H,5,7-8H2 |
| InchiKey:            | GNWCQWCBSQVEJR-WGIUUAEBSA-N                                                       |
| Formula:             | C15H22                                                                            |
| SMILES:              | CC1=CCC2C(C3=C(C)CCC13)C2(C)C                                                     |
| Mol. weight [g/mol]: | 202.34                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 251.30  | kJ/mol  | Joback Method  |
| hf            | -70.80  | kJ/mol  | Joback Method  |
| hfus          | 20.86   | kJ/mol  | Joback Method  |
| hvap          | 50.18   | kJ/mol  | Joback Method  |
| log10ws       | -4.53   |         | Crippen Method |
| logp          | 4.335   |         | Crippen Method |
| mcvol         | 181.030 | ml/mol  | McGowan Method |
| pc            | 2106.13 | kPa     | Joback Method  |
| rinpol        | 1533.00 |         | NIST Webbook   |
| tb            | 580.19  | K       | Joback Method  |
| tc            | 801.07  | K       | Joback Method  |
| tf            | 364.33  | K       | Joback Method  |
| vc            | 0.700   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 485.41 | J/mol×K | 580.19          | Joback Method |
| cpg           | 506.16 | J/mol×K | 617.00          | Joback Method |
| cpg           | 525.61 | J/mol×K | 653.82          | Joback Method |
| cpg           | 543.92 | J/mol×K | 690.63          | Joback Method |
| cpg           | 561.29 | J/mol×K | 727.44          | Joback Method |
| cpg           | 577.90 | J/mol×K | 764.26          | Joback Method |
| cpg           | 593.92 | J/mol×K | 801.07          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R407719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R407719&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                                     |

# 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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