

# (E,Z,Z)-1,5,9-Cyclododecatriene, 3-methyl

Inchi:

lnchl=1S/C12H18/c1-12-10-8-6-4-2-3-5-7-9-11-12/h2,4,7-10,12H,3,5-6,11H2,1H3/b4-2-,

InchiKey:

NONATMBHGBQNTN-DZNNNWEBSA-N

Formula:

C12H18

SMILES:

CC1C=CCC=CCCC=CC1

Mol. weight [g/mol]:

162.27

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 103.99  | kJ/mol  | Joback Method  |
| hf            | -94.15  | kJ/mol  | Joback Method  |
| hfus          | 11.84   | kJ/mol  | Joback Method  |
| hvap          | 44.47   | kJ/mol  | Joback Method  |
| log10ws       | -4.06   |         | Crippen Method |
| logp          | 3.865   |         | Crippen Method |
| mcvol         | 156.180 | ml/mol  | McGowan Method |
| pc            | 2679.08 | kPa     | Joback Method  |
| rinpol        | 1348.00 |         | NIST Webbook   |
| tb            | 512.34  | K       | Joback Method  |
| tc            | 751.10  | K       | Joback Method  |
| tf            | 217.06  | K       | Joback Method  |
| vc            | 0.558   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 347.15    | J/mol×K | 512.34          | Joback Method |
| cpg           | 449.93    | J/mol×K | 711.31          | Joback Method |
| cpg           | 432.11    | J/mol×K | 671.52          | Joback Method |
| cpg           | 412.92    | J/mol×K | 631.72          | Joback Method |
| cpg           | 392.37    | J/mol×K | 591.93          | Joback Method |
| cpg           | 370.44    | J/mol×K | 552.13          | Joback Method |
| cpg           | 466.39    | J/mol×K | 751.10          | Joback Method |
| dvisc         | 0.0000820 | Pa×s    | 512.34          | Joback Method |
| dvisc         | 0.0001333 | Pa×s    | 463.13          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002433 | Pa×s | 413.91 | Joback Method |
| dvisc | 0.0005225 | Pa×s | 364.70 | Joback Method |
| dvisc | 0.0014240 | Pa×s | 315.49 | Joback Method |
| dvisc | 0.0056226 | Pa×s | 266.27 | Joback Method |
| dvisc | 0.0413815 | Pa×s | 217.06 | Joback Method |

## Sources

|                        |                                                                                                                                       |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| <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>                 |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R2841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R2841&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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                                 |

Latest version available from:

<https://www.chemeo.com/cid/79-542-3/E-Z-Z-1-5-9-Cyclododecatriene-3-methyl.pdf>

Generated by Cheméo on 2025-12-05 08:27:33.074950927 +0000 UTC m=+4671450.604991581.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.