

# 2-Carene

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | (+)-2-Carene<br>(./-.)-2-Carene<br>3,7,7-Trimethylbicyclo[4.1.0]hept-2-ene<br>4-«delta»-carene<br>4-Â«deltaÂ»-carene<br>Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-<br>«delta»-2-Carene<br>«delta»-4-carene<br>Â«deltaÂ»-2-Carene<br>Â«deltaÂ»-4-carene |
| <b>Inchi:</b>               | InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h6,8-9H,4-5H2,1-3H3  |
| <b>InchiKey:</b>            | IBVJWOMJGCHRRW-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C10H16   |
| <b>SMILES:</b>              | CC1=CC2C(CC1)C2(C)C  |
| <b>Mol. weight [g/mol]:</b> | 136.23   |
| <b>CAS:</b>                 | 554-61-0   |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chl           | -6199.10 ± 2.30 | kJ/mol | NIST Webbook   |
| gf            | 149.85          | kJ/mol | Joback Method  |
| hf            | 25.00 ± 4.20    | kJ/mol | NIST Webbook   |
| hfl           | -22.60 ± 2.40   | kJ/mol | NIST Webbook   |
| hfus          | 11.43           | kJ/mol | Joback Method  |
| hvap          | 47.78           | kJ/mol | NIST Webbook   |
| hvap          | 47.60           | kJ/mol | NIST Webbook   |
| ie            | 8.26            | eV     | NIST Webbook   |
| ie            | 8.20            | eV     | NIST Webbook   |
| log10ws       | -2.93           |        | Crippen Method |
| logp          | 2.999           |        | Crippen Method |
| mcvol         | 125.740         | ml/mol | McGowan Method |
| pc            | 2890.51         | kPa    | Joback Method  |
| rinpol        | 1001.60         |        | NIST Webbook   |
| rinpol        | 996.47          |        | NIST Webbook   |
| rinpol        | 999.01          |        | NIST Webbook   |
| rinpol        | 1002.00         |        | NIST Webbook   |
| rinpol        | 993.75          |        | NIST Webbook   |

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|--------|---------|--------------|
| rinpol | 1001.00 | NIST Webbook |
| rinpol | 1002.00 | NIST Webbook |
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| rinpol | 1000.00 | NIST Webbook |
| rinpol | 1018.00 | NIST Webbook |
| rinpol | 1003.00 | NIST Webbook |
| rinpol | 1006.00 | NIST Webbook |
| rinpol | 1010.00 | NIST Webbook |
| rinpol | 1001.00 | NIST Webbook |
| rinpol | 1001.00 | NIST Webbook |
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| rinpol | 991.06  | NIST Webbook |
| rinpol | 994.00  | NIST Webbook |
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| rinpol | 984.00  | NIST Webbook |
| rinpol | 1001.00 | NIST Webbook |
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| rinpol | 984.00  | NIST Webbook |
| rinpol | 988.45  | NIST Webbook |
| rinpol | 1003.00 | NIST Webbook |

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|--------|---------|----------------------|---------------|
| rinpol | 1000.00 |                      | NIST Webbook  |
| rinpol | 1011.00 |                      | NIST Webbook  |
| rinpol | 994.00  |                      | NIST Webbook  |
| rinpol | 985.96  |                      | NIST Webbook  |
| rinpol | 1014.46 |                      | NIST Webbook  |
| rinpol | 1011.43 |                      | NIST Webbook  |
| rinpol | 1008.36 |                      | NIST Webbook  |
| rinpol | 1005.20 |                      | NIST Webbook  |
| rinpol | 1002.04 |                      | NIST Webbook  |
| rinpol | 1003.00 |                      | NIST Webbook  |
| rinpol | 1001.00 |                      | NIST Webbook  |
| ripol  | 1122.00 |                      | NIST Webbook  |
| ripol  | 1138.00 |                      | NIST Webbook  |
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| ripol  | 1142.00 |                      | NIST Webbook  |
| ripol  | 1110.00 |                      | NIST Webbook  |
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| ripol  | 1146.00 |                      | NIST Webbook  |
| ripol  | 1150.00 |                      | NIST Webbook  |
| ripol  | 1131.00 |                      | NIST Webbook  |
| ripol  | 1140.00 |                      | NIST Webbook  |
| ripol  | 1125.00 |                      | NIST Webbook  |
| ripol  | 1138.00 |                      | NIST Webbook  |
| ripol  | 1130.00 |                      | NIST Webbook  |
| tb     | 440.70  | K                    | NIST Webbook  |
| tc     | 654.83  | K                    | Joback Method |
| tf     | 267.76  | K                    | Joback Method |
| vc     | 0.484   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 274.36 | J/molxK | 445.66          | Joback Method |
| cpg           | 292.47 | J/molxK | 480.52          | Joback Method |
| cpg           | 309.23 | J/molxK | 515.38          | Joback Method |
| cpg           | 324.78 | J/molxK | 550.25          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 339.25 | J/mol×K | 585.11 | Joback Method |
| cpg | 352.77 | J/mol×K | 619.97 | Joback Method |
| cpg | 365.49 | J/mol×K | 654.83 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.42226e+01                   |
| Coeff. B                    | -3.62127e+03                  |
| Coeff. C                    | -6.36510e+01                  |
| Temperature range (K), min. | 323.52                        |
| Temperature range (K), max. | 470.03                        |

## Sources

|   |   |
|---|---|
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C554610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C554610&amp;Units=SI</a>   |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <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>hfl:</b>     | Liquid phase 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>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>pc:</b>     | Critical Pressure                   |
| <b>pvap:</b>   | Vapor pressure                      |
| <b>rinpol:</b> | Non-polar retention indices         |
| <b>ripol:</b>  | 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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