

# (+)-3-Carene

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (+)-«delta»3-Carene<br>(1S)-3,7,7-trimethylbicyclo[4.1.0]hept-3-ene<br>(1S,6R)-3,7,7-trimethylbicyclo[4.1.0]hept-3-ene<br>(1S,6R)-3-carene<br>3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene-, (1S,6R)-<br>Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-, (1S)-<br>Isodiprene |
| <b>Inchi:</b>               | InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9+/m1/s1  |
| <b>InchiKey:</b>            | BQOFWKZOCNGFEC-BDAKNGLRSA-N   |
| <b>Formula:</b>             | C10H16  |
| <b>SMILES:</b>              | CC1=CCC2C(C1)C2(C)C   |
| <b>Mol. weight [g/mol]:</b> | 136.23  |
| <b>CAS:</b>                 | 498-15-7  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | 149.85  | kJ/mol | Joback Method  |
| hf            | -69.08  | kJ/mol | Joback Method  |
| hfus          | 11.43   | kJ/mol | Joback Method  |
| hvap          | 48.50   | kJ/mol | 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        | 994.21  |        | NIST Webbook   |
| rinpol        | 1000.00 |        | NIST Webbook   |
| rinpol        | 1002.83 |        | NIST Webbook   |
| rinpol        | 1005.88 |        | NIST Webbook   |
| rinpol        | 1008.96 |        | NIST Webbook   |
| rinpol        | 995.00  |        | NIST Webbook   |
| rinpol        | 1025.31 |        | NIST Webbook   |
| rinpol        | 1010.00 |        | NIST Webbook   |
| rinpol        | 1012.09 |        | NIST Webbook   |
| rinpol        | 1012.09 |        | NIST Webbook   |
| rinpol        | 994.21  |        | NIST Webbook   |
| rinpol        | 1008.96 |        | NIST Webbook   |
| rinpol        | 1010.00 |        | NIST Webbook   |

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|--------|---------|----------------------|--|
| rinpol | 1021.88 |                      | NIST Webbook   |
| rinpol | 996.99  |                      | NIST Webbook   |
| rinpol | 1018.60 |                      | NIST Webbook   |
| rinpol | 1002.00 |                      | NIST Webbook   |
| rinpol | 1015.29 |                      | NIST Webbook   |
| rinpol | 995.00  |                      | NIST Webbook   |
| ripol  | 1148.00 |                      | NIST Webbook   |
| ripol  | 1148.00 |                      | NIST Webbook   |
| tb     | 442.63  | K                    | Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa |
| 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           | 339.25 | J/mol×K | 585.11          | Joback Method  |
| cpg           | 352.77 | J/mol×K | 619.97          | Joback Method  |
| cpg           | 274.36 | J/mol×K | 445.66          | Joback Method  |
| cpg           | 292.47 | J/mol×K | 480.52          | Joback Method  |
| cpg           | 309.23 | J/mol×K | 515.38          | Joback Method  |
| cpg           | 324.78 | J/mol×K | 550.25          | Joback Method  |
| cpg           | 365.49 | J/mol×K | 654.83          | Joback Method  |
| hvapt         | 42.80  | kJ/mol  | 401.00          | NIST Webbook   |
| pvap          | 101.33 | kPa     | 442.63          | Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 396.70 | K    | 26.70          | NIST Webbook |

## Sources

|  |   |
|--|---|
| Joback Method:   | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method:  | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:  | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C498157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C498157&amp;Units=SI</a> |
| Crippen Method:  | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method:  | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa | <a href="https://www.doi.org/10.1016/j.tca.2019.178318">https://www.doi.org/10.1016/j.tca.2019.178318</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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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