

# 3-Carene

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                            |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (.+-.)-3-carene<br>.DELTA.3-carene<br>3,7,7-Trimethylbicyclo[4.1.0]-3-heptene<br>3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene<br>3-Karen<br>3-Norcarene, 3,7,7-trimethyl-<br>3-«delta»-Carene<br>3-Â«deltaÂ»-Carene<br>4,7,7-Trimethyl-3-norcarene<br>Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-<br>Car-3-ene<br>Carene<br>delta-3-Carene<br>«DELTA»-car-3-ene<br>«delta» 3-carene<br>Â«DELTAÂ»-car-3-ene<br>Â«deltaÂ» 3-carene |
| Inchi:               | InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9+/m0/s1                                                                                                                                                                                                                                                                                                                                                 |
| InchiKey:            | BQOFWKZOCNGFEC-DTWKUNHWSA-N                                                                                                                                                                                                                                                                                                                                                                                                |
| Formula:             | C10H16                                                                                                                                                                                                                                                                                                                                                                                                                     |
| SMILES:              | CC1=CCC2C(C1)C2(C)C                                                                                                                                                                                                                                                                                                                                                                                                        |
| Mol. weight [g/mol]: | 136.23                                                                                                                                                                                                                                                                                                                                                                                                                     |
| CAS:                 | 13466-78-9                                                                                                                                                                                                                                                                                                                                                                                                                 |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chl           | -6192.20 ± 1.80 | kJ/mol | NIST Webbook   |
| gf            | 149.85          | kJ/mol | Joback Method  |
| hf            | 19.00 ± 4.00    | kJ/mol | NIST Webbook   |
| hfl           | -29.50 ± 1.90   | kJ/mol | NIST Webbook   |
| hfus          | 11.43           | kJ/mol | Joback Method  |
| hvap          | 48.50           | kJ/mol | NIST Webbook   |
| hvap          | 48.30 ± 3.10    | kJ/mol | NIST Webbook   |
| ie            | 8.40            | eV     | NIST Webbook   |
| ie            | 8.61            | eV     | NIST Webbook   |
| log10ws       | -2.93           |        | Crippen Method |
| logp          | 2.999           |        | Crippen Method |

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| mcvol  | 125.740 | ml/mol | McGowan Method |
| pc     | 2890.51 | kPa    | Joback Method  |
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| ripol | 1131.00       |         | NIST Webbook                                                                                                           |
| tb    | 442.62        | K       | Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Camphene, (+)-3-Carene, and (+-)-Limonene Systems |
| tb    | 442.00 ± 3.00 | K       | NIST Webbook                                                                                                           |
| tb    | 443.00 ± 4.00 | K       | NIST Webbook                                                                                                           |
| tb    | 446.50 ± 2.00 | K       | NIST Webbook                                                                                                           |
| tb    | 442.56        | K       | Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Camphene, (+)-3-Carene, and (+-)-Limonene Systems |
| tc    | 654.83        | K       | Joback Method                                                                                                          |
| tf    | 267.76        | K       | Joback Method                                                                                                          |
| vc    | 0.484         | m3/kmol | Joback Method                                                                                                          |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| 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           | 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                                                                                                                                                       |
| pvap | 101.33 | kPa     | 442.62 | Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Camphene, (+)-3-Carene, and (+-)-Limonene Systems                                              |
| pvap | 101.33 | kPa     | 442.56 | Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Camphene, (+)-3-Carene, and (+-)-Limonene Systems                                              |
| rhoI | 863.80 | kg/m3   | 298.15 | Measurement and correlation of vapor-liquid equilibrium data for binary and ternary systems composed of (-)-beta-caryophyllene, p-cymene and 3-carene at 101.33 kPa |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 441.70 | K    | 94.00          | NIST Webbook |

## Correlations

| Information   | Value                   |
|---------------|-------------------------|
| Property code | pvap                    |
| Equation      | ln(Pvp) = A + B/(T + C) |
| Coeff. A      | 1.33597e+01             |
| Coeff. B      | -3.18950e+03            |
| Coeff. C      | -8.16270e+01            |

|                             |        |
|-----------------------------|--------|
| Temperature range (K), min. | 325.62 |
| Temperature range (K), max. | 477.92 |

## Sources

Measurement and correlation of vapor-liquid equilibrium data for binary and ternary systems composed of isobutane, propylene, and (+)-limonene systems: McGowan Method:

<https://www.doi.org/10.1016/j.jct.2018.08.015>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13466789&Units=SI>

The Yaws Handbook of Vapor Pressure: Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

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

## 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>rho:</b>     | Liquid Density                                            |
| <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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