

# p-Cymene

|                      |                                                      |
|----------------------|------------------------------------------------------|
| Other names:         | 1-(1-methylethyl)-4-methylbenzene                    |
|                      | 1-Isopropyl-4-methylbenzene                          |
|                      | 1-METHYL-4-ISOPROPYLBENZENE                          |
|                      | 1-Methyl-4-(1-methylethyl)-benzene                   |
|                      | 2-p-Tolylpropane                                     |
|                      | 4-Isopropyl-1-methylbenzene                          |
|                      | 4-Isopropyltoluene                                   |
|                      | 4-Methylisopropylbenzene                             |
|                      | Benzene, 1-isopropyl-4-methyl-                       |
|                      | Benzene, 1-methyl-4-(1-methylethyl)-                 |
|                      | Camphogen                                            |
|                      | Cumene, p-methyl-                                    |
|                      | Cymene                                               |
|                      | Cymol                                                |
|                      | Dolcymene                                            |
|                      | NSC 4162                                             |
|                      | P-ISOPROPYL TOLUENE                                  |
|                      | P-METHYL CUMENE                                      |
|                      | Paracymene                                           |
|                      | Paracymol                                            |
|                      | benzene, 1-(1-methylethyl)-4-methyl-                 |
|                      | benzene, 1-methyl-4-methylethyl-                     |
|                      | p-Cimene                                             |
|                      | p-Cymol                                              |
|                      | p-Isopropylmethylbenzene                             |
|                      | p-Isopropyltoluene                                   |
|                      | p-Mentha-1,3,5-triene                                |
|                      | p-Methylcumene                                       |
|                      | p-Methylisopropylbenzene                             |
| Inchi:               | InChI=1S/C10H14/c1-8(2)10-6-4-9(3)5-7-10/h4-8H,1-3H3 |
| InchiKey:            | HFPZCAJZSCWRBC-UHFFFAOYSA-N                          |
| Formula:             | C10H14                                               |
| SMILES:              | <chem>Cc1ccc(C(C)C)cc1</chem>                        |
| Mol. weight [g/mol]: | 134.22                                               |
| CAS:                 | 99-87-6                                              |

## Physical Properties

| Property code | Value           | Unit   | Source                      |
|---------------|-----------------|--------|-----------------------------|
| af            | 0.3730          |        | KDB                         |
| chl           | -5857.90 ± 1.00 | kJ/mol | NIST Webbook                |
| chl           | -5857.60 ± 2.20 | kJ/mol | NIST Webbook                |
| dm            | 0.00            | debye  | KDB                         |
| gf            | 133.66          | kJ/mol | Joback Method               |
| hcg           | 5865.55         | kJ/mol | KDB                         |
| hcn           | 5558.026        | kJ/mol | KDB                         |
| hf            | -29.95          | kJ/mol | Joback Method               |
| hfl           | -78.00 ± 1.10   | kJ/mol | NIST Webbook                |
| hfl           | -78.40 ± 2.10   | kJ/mol | NIST Webbook                |
| hfus          | 11.79           | kJ/mol | Joback Method               |
| hvap          | 48.90           | kJ/mol | NIST Webbook                |
| hvap          | 49.20           | kJ/mol | NIST Webbook                |
| hvap          | 50.30           | kJ/mol | NIST Webbook                |
| ie            | 8.29            | eV     | NIST Webbook                |
| ie            | 8.29            | eV     | NIST Webbook                |
| log10ws       | -3.77           |        | Estimated Solubility Method |
| logp          | 3.118           |        | Crippen Method              |
| mcvol         | 128.000         | ml/mol | McGowan Method              |
| nfpaf         | %!d(float64=2)  |        | KDB                         |
| nfpah         | %!d(float64=2)  |        | KDB                         |
| pc            | 2800.00         | kPa    | KDB                         |
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| sl    | 306.70        | J/mol×K | NIST Webbook                                                                                                                                                                         |
| tb    | 448.00 ± 2.00 | K       | NIST Webbook                                                                                                                                                                         |
| tb    | 449.70        | 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 |
| tb    | 449.39        | K       | Measurement and Correlation of Vapor-Liquid Equilibrium Data for ss-Pinene + p-Cymene + (S)-(-)-Limonene at Atmospheric Pressure                                                     |
| tb    | 450.30        | K       | NIST Webbook                                                                                                                                                                         |
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| tf | 203.02 ± 2.00 | K       | NIST Webbook                                                                                       |
| tf | 204.20        | K       | KDB                                                                                                |
| tf | 203.95 ± 0.70 | K       | NIST Webbook                                                                                       |
| tf | 205.45 ± 0.70 | K       | NIST Webbook                                                                                       |
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| tf | 205.19 ± 0.03 | K       | NIST Webbook                                                                                       |
| tf | 205.17 ± 0.05 | K       | NIST Webbook                                                                                       |
| tf | 204.60        | K       | Solid-Liquid Equilibria in Binary Mixtures of 1,8-Cineole with p-Cymene, beta-Pinene, and Camphene |
| tt | 204.20 ± 0.30 | K       | NIST Webbook                                                                                       |
| vc | 0.481         | m3/kmol | Joback Method                                                                                      |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 336.48    | J/mol×K | 670.22          | Joback Method |
| cpg           | 325.13    | J/mol×K | 635.09          | Joback Method |
| cpg           | 257.41    | J/mol×K | 459.42          | Joback Method |
| cpg           | 272.52    | J/mol×K | 494.55          | Joback Method |
| cpg           | 286.82    | J/mol×K | 529.69          | Joback Method |
| cpg           | 300.33    | J/mol×K | 564.82          | Joback Method |
| cpg           | 313.10    | J/mol×K | 599.96          | Joback Method |
| cpl           | 236.40    | J/mol×K | 297.10          | NIST Webbook  |
| cpl           | 242.30    | J/mol×K | 298.00          | NIST Webbook  |
| dvisc         | 0.0005277 | Pa×s    | 342.91          | Joback Method |
| dvisc         | 0.0008475 | Pa×s    | 304.07          | Joback Method |
| dvisc         | 0.0015637 | Pa×s    | 265.24          | Joback Method |
| dvisc         | 0.0002060 | Pa×s    | 459.42          | Joback Method |
| dvisc         | 0.0002660 | Pa×s    | 420.58          | Joback Method |
| dvisc         | 0.0003618 | Pa×s    | 381.75          | Joback Method |
| dvisc         | 0.0035598 | Pa×s    | 226.40          | Joback Method |
| hfust         | 9.67      | kJ/mol  | 204.20          | NIST Webbook  |
| hfust         | 9.67      | kJ/mol  | 204.20          | NIST Webbook  |
| hfust         | 9.66      | kJ/mol  | 204.20          | NIST Webbook  |
| hvapt         | 44.00     | kJ/mol  | 416.00          | NIST Webbook  |

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|------|---------|-------|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| pvap | 101.33  | kPa   | 449.70 | 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 |
| pvap | 100.70  | kPa   | 449.39 | Measurement and correlation of (vapor + liquid) equilibrium data for {alpha-pinene + p-cymene + (S)-(-)-limonene} ternary system at atmospheric pressure                             |
| rfi  | 1.47890 |       | 318.15 | Excess Molar Enthalpies of p-Cymene + r-Pinene + a-Pinene at (298.15, 308.15, and 318.15) K and at Atmospheric Pressure                                                              |
| rfi  | 1.48310 |       | 308.15 | Excess Molar Enthalpies of p-Cymene + r-Pinene + a-Pinene at (298.15, 308.15, and 318.15) K and at Atmospheric Pressure                                                              |
| rfi  | 1.48780 |       | 298.15 | Excess Molar Enthalpies of p-Cymene + r-Pinene + a-Pinene at (298.15, 308.15, and 318.15) K and at Atmospheric Pressure                                                              |
| rfi  | 1.48850 |       | 298.15 | KDB                                                                                                                                                                                  |
| rhoI | 853.24  | kg/m3 | 298.20 | Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K                                                                       |

|      |        |       |        |                                                                                                                                                   |
|------|--------|-------|--------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| rhoI | 852.99 | kg/m3 | 298.15 | Thermophysical and volumetric study of mixtures {p-cymene + propan-1-ol} at several temperatures and atmospheric pressure. Modeling with COSMO-RS |
| rhoI | 828.69 | kg/m3 | 328.15 | Isobaric molar heat capacities of the mixture (p-cymene + ethanol) at several temperatures and atmospheric pressure                               |
| rhoI | 836.81 | kg/m3 | 318.15 | Isobaric molar heat capacities of the mixture (p-cymene + ethanol) at several temperatures and atmospheric pressure                               |
| rhoI | 844.94 | kg/m3 | 308.15 | Thermophysical and volumetric study of mixtures {p-cymene + propan-1-ol} at several temperatures and atmospheric pressure. Modeling with COSMO-RS |
| rhoI | 844.89 | kg/m3 | 308.15 | Isobaric molar heat capacities of the mixture (p-cymene + ethanol) at several temperatures and atmospheric pressure                               |
| rhoI | 852.93 | kg/m3 | 298.15 | Isobaric molar heat capacities of the mixture (p-cymene + ethanol) at several temperatures and atmospheric pressure                               |
| rhoI | 857.00 | kg/m3 | 293.00 | KDB                                                                                                                                               |

|       |        |         |        |                                                                                                                                                                     |
|-------|--------|---------|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| rho1  | 836.86 | kg/m3   | 318.15 | Thermophysical and volumetric study of mixtures {p-cymene + propan-1-ol} at several temperatures and atmospheric pressure. Modeling with COSMO-RS                   |
| rho1  | 828.75 | kg/m3   | 328.15 | Thermophysical and volumetric study of mixtures {p-cymene + propan-1-ol} at several temperatures and atmospheric pressure. Modeling with COSMO-RS                   |
| rho1  | 853.20 | 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 |
| sfust | 47.30  | J/mol×K | 204.20 | NIST Webbook                                                                                                                                                        |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.46754e+01                   |
| Coeff. B                    | -3.85578e+03                  |
| Coeff. C                    | -6.61110e+01                  |
| Temperature range (K), min. | 334.10                        |
| Temperature range (K), max. | 477.88                        |

| Information   | Value                                                  |
|---------------|--------------------------------------------------------|
| Property code | pvap                                                   |
| Equation      | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A      | 1.06198e+02                                            |

|                             |              |
|-----------------------------|--------------|
| Coeff. B                    | -9.64396e+03 |
| Coeff. C                    | -1.33601e+01 |
| Coeff. D                    | 7.19714e-06  |
| Temperature range (K), min. | 205.25       |
| Temperature range (K), max. | 653.15       |

## Sources

High-Pressure Vapor-Liquid Equilibria for a CO<sub>2</sub> + p-Cymene Binary System at Temperatures from 315.15 to 353.15 K: <https://www.doi.org/10.1021/acs.jced.9b00664>  
[http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

Relation between characteristic molecular volume and hydrophobicity of nonpolar molecules: <https://www.doi.org/10.1016/j.jct.2010.04.011>  
<http://link.springer.com/article/10.1007/BF02311772>

Thermodynamics of solvation in propylene glycol and methyl cellosolve method: <https://www.doi.org/10.1016/j.jct.2014.06.006>  
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The Yaws Handbook of Vapor Pressure: Determination and Correlation of Solubility of Borneol, Camphor, and Isoborneol in Different Solvents: <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<https://www.doi.org/10.1021/acs.jced.9b00045>  
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Isobaric molar heat capacities of the mixture (p-cymene + ethanol) at several temperatures and correlation of vapor-liquid equilibrium data for binary systems composed of p-cymene, constant-boiling azeotropic mixtures, p-cymene and p-methylphenol at 101.33 kPa, mixtures of 1,8-Cineole with p-Cymene, 8-epi-pinane, and thymol with p-Cymene + r-Pinene + α-Pinene at (298.15, 308.15, and 318.15) K and xerosephic study of mixtures {p-cymene + propan-1-ol} at several temperatures and correlation of Vapor-Liquid Equilibrium Data: <https://www.doi.org/10.1016/j.jct.2017.03.027>  
<https://www.doi.org/10.1016/j.tca.2019.178318>  
<https://www.doi.org/10.1021/je3010535>  
<https://www.doi.org/10.1021/je900653p>  
<https://www.doi.org/10.1021/je060420p>  
<https://www.doi.org/10.1016/j.jct.2018.03.021>  
<https://www.doi.org/10.1021/je101151f>  
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C99876&Units=SI>  
<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=674>

Measurement and correlation of (vapor + liquid) equilibrium data for p-cymene and correlation of vapor-liquid equilibrium data for binary systems composed of p-cymene, constant-boiling azeotropic mixtures, p-cymene and p-methylphenol at 101.33 kPa, mixtures of 1,8-Cineole with p-Cymene, 8-epi-pinane, and thymol with p-Cymene + r-Pinene + α-Pinene at (298.15, 308.15, and 318.15) K and xerosephic study of mixtures {p-cymene + propan-1-ol} at several temperatures and correlation of Vapor-Liquid Equilibrium Data: <https://www.doi.org/10.1016/j.jct.2012.10.017>  
<https://www.doi.org/10.1016/j.jct.2018.08.015>  
<https://www.doi.org/10.1016/j.jct.2015.04.020>  
<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=674>  
<https://www.doi.org/10.1021/acs.jced.8b00086>

Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K:

## Legend

|      |                                        |
|------|----------------------------------------|
| af:  | Acentric Factor                        |
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity                |
| cpl: | Liquid phase heat capacity             |

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>dm:</b>      | Dipole Moment                                             |
| <b>dvisc:</b>   | Dynamic viscosity                                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation                   |
| <b>hcg:</b>     | Heat of Combustion, Gross form                            |
| <b>hcn:</b>     | Heat of Combustion, Net Form                              |
| <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>hfust:</b>   | Enthalpy of fusion at a given temperature                 |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions           |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature           |
| <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>nfpaf:</b>   | NFPA Fire Rating                                          |
| <b>nfpah:</b>   | NFPA Health Rating                                        |
| <b>pc:</b>      | Critical Pressure                                         |
| <b>pvap:</b>    | Vapor pressure                                            |
| <b>rfi:</b>     | Refractive Index                                          |
| <b>rho:</b>     | Liquid Density                                            |
| <b>rinpol:</b>  | Non-polar retention indices                               |
| <b>ripol:</b>   | Polar retention indices                                   |
| <b>sfust:</b>   | Entropy of fusion at a given temperature                  |
| <b>sl:</b>      | Liquid phase molar entropy at standard conditions         |
| <b>tb:</b>      | Normal Boiling Point Temperature                          |
| <b>tc:</b>      | Critical Temperature                                      |
| <b>tf:</b>      | Normal melting (fusion) point                             |
| <b>tt:</b>      | Triple Point Temperature                                  |
| <b>vc:</b>      | Critical Volume                                           |

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