# Eucalyptol

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|---|---|
| **Other names:** | 1,3,3-Trimethyl-2-oxabicyclo[2,2,2]octan |
| | 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane |
| | 1,8-Cineol |
| | 1,8-Cineole |
| | 1,8-Cineole (eucalyptol) |
| | 1,8-Epoxy-p-menthane |
| | 1,8-Oxido-p-menthane |
| | 1,8-cineol (eucalyptol) |
| | 2-Oxa-1,3,3-trimethylbicyclo[2.2.2]octane |
| | 2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- |
| | Cajeputol |
| | Cineol |
| | Cineole |
| | Cucalyptol |
| | Eucalyptole |
| | Eucapur |
| | Eukalyptol |
| | NCI-C56575 |
| | NSC 6171 |
| | Terpan |
| | Zineol |
| | p-Cineole |
| | p-Menthane, 1,8-epoxy- |
| **Inchi:** | InChI=1S/C10H18O/c1-9(2)8-4-6-10(3,11-9)7-5-8/h8H,4-7H2,1-3H3 |
| **InchiKey:** | WEEGYLXZBRQIMU-UHFFFAOYSA-N |
| **Formula:** | C10H18O |
| **SMILES:** | CC12CCC(CC1)C(C)(C)O2 |
| **Mol. weight [g/mol]:** | 154.25 |
| **CAS:** | 470-82-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 25.81 | kJ/mol | Joback Method |
| hf | -238.31 | kJ/mol | Joback Method |
| hfus | 10.18 | kJ/mol | Joback Method |
| hvap | 49.00 | kJ/mol | NIST Webbook |

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| hvap | 53.20 | kJ/mol | NIST Webbook |
| log10ws | -1.64 | | Estimated Solubility Method |
| log10ws | -1.72 | | Aqueous Solubility Prediction Method |
| logp | 2.744 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 3018.96 | kPa | Joback Method |
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# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
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| cpg | 421.37 | J/mol×K | 695.50 | Joback Method |
| cpg | 392.78 | J/mol×K | 621.33 | Joback Method |
| cpg | 407.45 | J/mol×K | 658.42 | Joback Method |
| cpg | 321.67 | J/mol×K | 472.98 | Joback Method |
| cpg | 341.80 | J/mol×K | 510.07 | Joback Method |
| cpg | 360.20 | J/mol×K | 547.15 | Joback Method |
| cpg | 377.11 | J/mol×K | 584.24 | Joback Method |
| hvapt | 35.60 | kJ/mol | 283.50 | NIST Webbook |
| hvapt | 41.10 | kJ/mol | 378.00 | NIST Webbook |
| pvap | 0.13 | kPa | 288.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.83 | kPa | 318.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 1.10 | kPa | 323.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 0.07 | kPa | 278.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.09 | kPa | 283.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.63 | kPa | 313.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |

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|---|---|---|---|---|
| pvap | 0.18 | kPa | 293.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.25 | kPa | 298.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.35 | kPa | 303.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.48 | kPa | 308.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.63 | kPa | 313.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 0.83 | kPa | 318.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |
| pvap | 1.10 | kPa | 323.15 | Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K |

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|---|---|---|---|---|
| pvap | 1.33 | kPa | 326.65 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 2.67 | kPa | 341.55 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 5.33 | kPa | 357.25 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 6.67 | kPa | 363.45 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 13.33 | kPa | 381.45 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |

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|---|---|---|---|---|
| pvap | 20.00 | kPa | 392.75 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 26.66 | kPa | 401.75 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 33.33 | kPa | 408.65 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 40.00 | kPa | 414.65 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 0.25 | kPa | 298.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |

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|---|---|---|---|---|
| pvap | 53.33 | kPa | 424.65 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 60.00 | kPa | 428.85 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 66.66 | kPa | 432.75 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 73.33 | kPa | 436.35 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 79.99 | kPa | 439.75 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |

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|---|---|---|---|---|
| pvap | 86.66 | kPa | 442.85 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 93.33 | kPa | 445.85 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 99.61 | kPa | 448.65 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 101.33 | kPa | 449.15 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |
| pvap | 0.07 | kPa | 278.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |

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|---|---|---|---|---|
| pvap | 0.09 | kPa | 283.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.13 | kPa | 288.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.18 | kPa | 293.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.25 | kPa | 298.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.35 | kPa | 303.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.48 | kPa | 308.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.48 | kPa | 308.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |

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|---|---|---|---|---|
| pvap | 0.83 | kPa | 318.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 1.10 | kPa | 323.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| pvap | 0.07 | kPa | 278.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 0.09 | kPa | 283.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 0.13 | kPa | 288.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 0.18 | kPa | 293.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 46.66 | kPa | 419.95 | P, rho, T Measurements and Isobaric Vapor-Liquid-Equilibria of the 1,3,3-Trimethyl-2-oxabicycle[2,2,2]octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis |

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|---|---|---|---|---|
| pvap | 0.35 | kPa | 303.15 | Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K |
| pvap | 0.63 | kPa | 313.15 | Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K |
| rfi | 1.45531 | | 298.15 | Thermophysical properties of the binary mixtures (1,8-cineole + 1-alkanol) at T = (298.15 and 313.15) K and at atmospheric pressure |
| rfi | 1.44834 | | 313.15 | Thermophysical properties of the binary mixtures (1,8-cineole + 1-alkanol) at T = (298.15 and 313.15) K and at atmospheric pressure |
| rhol | 920.51 | kg/m3 | 298.15 | Molar heat capacities of the mixture {1,8-cineole + ethanol} at several temperatures and atmospheric pressure |
| rhol | 924.84 | kg/m3 | 293.15 | (Liquid + liquid) equilibria of four alcohol-water systems containing 1,8-cineole at T = 298.15 K |
| rhol | 920.68 | kg/m3 | 298.15 | Isobaric VLE of the mixture {1,8-cineole + ethanol}. EOS analysis and COSMO-RS modeling |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.48351e+01 |
| Coeff. B | -4.19031e+03 |
| Coeff. C | -3.94100e+01 |
| Temperature range (K), min. | 327.45 |
| Temperature range (K), max. | 479.40 |

# Datasets

## Mass density, kg/m3

| Pressure, kPa - Liquid | Temperature, K - Liquid | Mass density, kg/m3 - Liquid |
|---|---|---|
| 100.00 | 293.15 | 924.84 |

Reference *https://www.doi.org/10.1016/j.jct.2016.12.018*

| Temperature, K | Pressure, kPa | Mass density, kg/m3 |
|---|---|---|
| 283.15 | 100.00 | 933.3 |
| 283.15 | 5000.00 | 936.7 |
| 283.15 | 10000.00 | 939.9 |
| 283.15 | 15000.00 | 943.1 |
| 283.15 | 20000.00 | 946.2 |
| 298.15 | 100.00 | 920.4 |
| 298.15 | 5000.00 | 924.1 |
| 298.15 | 10000.00 | 927.7 |
| 298.15 | 15000.00 | 931.2 |
| 298.15 | 20000.00 | 934.4 |
| 313.15 | 100.00 | 907.3 |
| 313.15 | 5000.00 | 911.4 |
| 313.15 | 10000.00 | 915.2 |
| 313.15 | 15000.00 | 919.0 |
| 313.15 | 20000.00 | 922.5 |

# Sources

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|---|---|
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| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Molar heat capacities of the mixture {1,8-cineole + ethanol} at several temperatures and atmospheric pressure:** | https://www.doi.org/10.1016/j.jct.2015.09.012 |
| **Solid-Liquid Equilibria in Binary Mixtures of 1,8-Cineole with p-Cymene, beta-Pinene, and Camphene:** | https://www.doi.org/10.1021/je900653p |
| **Thermophysical properties of the binary mixtures (1,8-cineole + 1-alkanol) at T = (298.15 and 313.15) K and at atmospheric pressure:** | https://www.doi.org/10.1016/j.jct.2009.08.016 |
| **(Liquid + liquid) extraction of phenolic from aqueous solutions with cineole:** | https://www.doi.org/10.1016/j.jct.2016.12.018 |
| **Total vapour pressure and excess Gibbs energy of ethanol with 1,8-cineole at temperatures between 278.15 K and 323.15 K:** | https://www.doi.org/10.1016/j.fluid.2011.07.002 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K:** | https://www.doi.org/10.1021/je200011e |
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| **(Liquid + liquid) equilibria of four alcohol-water systems containing 1,8-cineole at T = 298.15 K:** | https://www.doi.org/10.1016/j.jct.2016.06.010 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
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| **Setup and Validation of a PGT Measuring Device. Volumetric Behavior of the Mixture 1,8-Cineole + Ethanol:** | https://www.doi.org/10.1021/je800024u |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
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| **Vapor Pressures and Activity Coefficients of (1-Propanol + 1,8-Cineole) at 10 Temperatures between 278.15 K and 323.15 K:** | https://www.doi.org/10.1021/je300736k |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |

| | |
|---|---|
| **rfi:** | Refractive Index |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |