Eucalyptol

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

hvap	53.20	kJ/mol	NIST Webbook
log10ws	-1.72		Aqueous Solubility Prediction Method
log10ws	-1.64		Estimated Solubility Method
logp	2.744		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1023.90		NIST Webbook
rinpol	1006.89		NIST Webbook
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ripol	1212.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1176.00		NIST Webbook
tb	449.50 ± 0.50	K	NIST Webbook
tb	449.15	K	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
tb	449.60	K	NIST Webbook
tb	449.15 ± 1.50	K	NIST Webbook
tb	449.50 ± 0.35	K	NIST Webbook
tb	449.50 ± 0.50	K	NIST Webbook
tb	449.50 ± 0.50	K	NIST Webbook
tc	695.50	K	Joback Method
tf	274.63 ± 0.10	K	NIST Webbook
tf	274.40	K	Solid-Liquid Equilibria in Binary Mixtures of 1,8-Cineole with p-Cymene, beta-Pinene, and Camphene
tf	274.40	K	Aqueous Solubility Prediction Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	392.78	J/mol×K	621.33	Joback Method
cpg	360.20	J/mol×K	547.15	Joback Method
cpg	377.11	J/mol×K	584.24	Joback Method
cpg	421.37	J/mol×K	695.50	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
hvapt	35.60	kJ/mol	283.50	NIST Webbook
hvapt	41.10	kJ/mol	378.00	NIST Webbook
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	0.35	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	0.48	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
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
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	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

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	0.13	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	0.18	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
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
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	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	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	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
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
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
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	0.63	kPa	313.15	Isothermal Vapor-Liquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K
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	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	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	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
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
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
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
rhol	920.51	kg/m3	298.15	Molar heat capacities of the mixture {1,8-cineole + ethanol} at several temperatures and atmospheric pressure

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

Reference *https://www.doi.org/10.1021/je800024u*

Sources

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Thermophysical properties of the binary mixtures (1,8-cineole + 1-alkanol) at T = (298.15 and 313.15) K https://www.doi.org/10.1016/j.jct.2009.08.016

Solid−Liquid Equilibria in Binary Mixtures of 1,8-Cineole with p-Cymene, α-Pinene, and Camphene: https://www.doi.org/10.1021/je900653p

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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

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