Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-

Other names: (+)-(4R)-limonene
(+)-.alpha.-limonene
(+)-4-isopropenyl-1-methylcyclohexene
(+)-dipentene
(+)-limonene
(+)-p-mentha-1,8-diene
(-)-Limonene
(4R)-(+)-limonene
(R)-(+)-limonene
(R)-(+)-p-mentha-1,8-diene
(R)-1-methyl-4-(1-methylethenyl)cyclohexene
(R)-4-isopropenyl-1-methyl-1-cyclohexene
(R)-limonene
(R)-p-mentha-1,8-diene
(S)-p-mentha-1,8-diene
D-(+)-limonene
D-limonene
L-Limonene
Limonene
carvene
cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)-,
limonene, (+)-
p-Mentha-1,8-diene, (S)-(-)-
p-mentha-1,8-diene, (R)-(+)-

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m0/s1

InchiKey: XMGQYMWWDOXHJM-JTQLQIEISA-N

Formula: C10H16

SMILES: C=C(C)C1CC=C(C)CC1

Mol. weight [g/mol]: 136.23

CAS: 5989-54-8

Physical Properties

Property code	Value	Unit	Source
gf	157.39	kJ/mol	Joback Method
hf	-33.46	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method

hvap	49.00 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1020.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1193.00		NIST Webbook
tb	449.40 ± 2.00	K	NIST Webbook
tb	449.00 ± 4.00	K	NIST Webbook
tb	450.00 ± 6.00	K	NIST Webbook
tb	449.40 ± 3.00	K	NIST Webbook
tb	449.20	K	NIST Webbook
tc	657.16	K	Joback Method
tf	207.40	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.80	J/mol×K	448.45	Joback Method
cpg	304.13	J/mol×K	518.02	Joback Method
cpg	319.94	J/mol×K	552.80	Joback Method
cpg	334.90	J/mol×K	587.59	Joback Method
cpg	349.03	J/mol×K	622.37	Joback Method
cpg	362.36	J/mol×K	657.16	Joback Method
cpg	287.42	J/mol×K	483.23	Joback Method

dvisc	0.0004520	Pa×s	353.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0004130	Pa×s	363.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0003820	Pa×s	373.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0010780	Pa×s	283.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	

dvisc	0.0009320	Pa×s	293.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0005000	Pa×s	343.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0008160	Pa×s	303.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0007220	Pa×s	313.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	

dvisc	0.0006450	Pa×s	323.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0005800	Pa×s	333.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0005240	Pa×s	343.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0005660	Pa×s	333.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	

dvisc	0.0006280	Pa×s	323.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0007020	Pa×s	313.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0007930	Pa×s	303.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
dvisc	0.0008900	Pa×s	298.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	

dvisc	0.0008970	Pa×s	298.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0004760	Pa×s	353.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure	
dvisc	0.0009020	Pa×s	293.15	Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene] over the complete concentration range, at different temperatures	
hvapt	45.50	kJ/mol	333.00	NIST Webbook	
hvapt	47.00	kJ/mol	387.50	NIST Webbook	
rfi	1.47300		293.20	Vapor Liquid Equilibrium Data for Binary Systems of 1-Methyl-4-(1-methylethenyl)-cyclohexene + {Ethanol, Propan-1-ol, Propan-2-ol, Butan-1-ol, Pentan-1-ol, or Hexan-1-ol} at 40 kPa	

rfi	1.47081		298.15	Deterpenation of Citrus Essential Oil by Liquid-Liquid Extraction with 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide Ionic Liquids	
rhol	837.31	kg/m3	298.15	Ternary and quaternary (liquid + liquid) equilibria for (water + ethanol + a-pinene, +b-pinene, or +limonene) and (water + ethanol + a-pinene + limonene) at the temperature 298.15 K	
rhol	838.68	kg/m3	298.15	Improved concentration of citrus essential oil by solvent extraction with acetate ionic liquids	
rhol	837.31	kg/m3	298.15	Temperature dependence on mutual solubility of binary (methanol + limonene) mixture and (liquid + liquid) equilibria of ternary (methanol + ethanol + limonene) mixture	
rhol	840.73	kg/m3	298.20	Deterpenation of Citrus Essential Oils Using Glycerol-Based Deep Eutectic Solvents	
rhol	841.35	kg/m3	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K	
rhol	837.31	kg/m3	298.15	Mutual Solubilities of Terpene in Methanol and Water and Their Multicomponent Liquid-Liquid Equilibria	

rhol	841.35	kg/m3	298.20	Fractionation of orange essential oil using liquid-liquid extraction: Equilibrium data for model and real systems at 298.2 K.

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35555e+01
Coeff. B	-3.43704e+03
Coeff. C	-6.65700e+01
Temperature range (K), min.	325.62
Temperature range (K), max.	483.49

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	20000.00	862.0
283.15	25000.00	864.9
283.15	30000.00	867.7
283.15	35000.00	870.4
283.15	40000.00	873.3
298.15	20000.00	851.5
298.15	25000.00	854.5
298.15	30000.00	857.6
298.15	35000.00	860.9
298.15	40000.00	863.4
313.15	20000.00	841.0
313.15	25000.00	844.2
313.15	30000.00	847.2

313.15	35000.00	850.3
313.15	40000.00	853.3
328.15	20000.00	830.5
328.15	25000.00	833.8
328.15	30000.00	837.2
328.15	35000.00	840.4
328.15	40000.00	843.8
343.15	20000.00	820.1
343.15	25000.00	823.7
343.15	30000.00	827.3
343.15	35000.00	831.1
343.15	40000.00	834.6
358.15	20000.00	810.2
358.15	25000.00	813.9
358.15	30000.00	817.6
358.15	35000.00	821.3
358.15	40000.00	824.8

Reference *https://www.doi.org/10.1016/j.jct.2011.12.013*

Pressure, kPa	Temperature, K	Mass density, kg/m3
100.00	298.20	838.59

Reference *https://www.doi.org/10.1016/j.jct.2013.09.044*

Pressure, kPa	Temperature, K	Mass density, kg/m3
101.80	298.15	838.59

Reference *https://www.doi.org/10.1016/j.jct.2013.11.026*

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	839.1

Reference *https://www.doi.org/10.1021/acs.jced.8b00939*

Temperature, K	Pressure, kPa	Mass density, kg/m3
283.15	20000.00	862.0
283.15	25000.00	864.9
283.15	30000.00	867.7
283.15	35000.00	870.4

283.15	40000.00	873.3
298.15	20000.00	851.5
298.15	25000.00	854.5
298.15	30000.00	857.6
298.15	35000.00	860.9
298.15	40000.00	863.4
313.15	20000.00	841.0
313.15	25000.00	844.2
313.15	30000.00	847.2
313.15	35000.00	850.3
313.15	40000.00	853.3
328.15	20000.00	830.5
328.15	25000.00	833.8
328.15	30000.00	837.2
328.15	35000.00	840.4
328.15	40000.00	843.8
343.15	20000.00	820.1
343.15	25000.00	823.7
343.15	30000.00	827.3
343.15	35000.00	831.1
343.15	40000.00	834.6
358.15	20000.00	810.2
358.15	25000.00	813.9
358.15	30000.00	817.6
358.15	35000.00	821.3
358.15	40000.00	824.8

Reference *https://www.doi.org/10.1021/je1009619*

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McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
(Liquid + liquid) equilibria of (water + linalool + limonene) ternary system at T = (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1016/j.jct.2008.06.012
Improved concentration of citrus essential oil by solvent extraction with acetate ionic liquids:	https://www.doi.org/10.1016/j.fluid.2013.10.036
Density, viscosity, vapour liquid equilibrium, excess molar enthalpy, and their correlations of the binary system [1-pentanol + R-(+)-limonene]	https://www.doi.org/10.1016/j.fluid.2010.03.001
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Temperature dependence on mutual solubility of binary (methanol + limonene) mixtures and (liquid + liquid) equilibria for (water + methanol + limonene) ternary systems at different temperatures:	https://www.doi.org/10.1016/j.jct.2008.10.013
Measurement of activity coefficients at infinite dilution for acetonitrile, water, and 1-methylimidazole in (water + acetonitrile + limonene) at the temperature 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.018
Vapor−Liquid Equilibria Measurements of Bitter Orange Aroma Compounds Highly Diluted in Boiling Hydro-Alcoholic Solutions at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2008.09.011
	https://www.doi.org/10.1021/je3004854

Vapor Liquid Equilibrium Data for Binary Systems of 1-Methyl-4-(1-methylethenyl)-cyclohexene + {Ethanol, Propan-1-ol, Propan-2-ol, Butan-1-ol, Pentan-1-ol, or Hexan-1-ol} at 40 kPa:	https://www.doi.org/10.1021/je300347z
Deterpenation of Citrus Essential Oil by Liquid-Liquid Extraction with 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide Ionic Liquids:	https://www.doi.org/10.1021/je1011339
(Ternary liquid + liquid) equilibria for (water + acetone + alpha-pinene or beta-pinene, or limonene) mixtures:	https://www.doi.org/10.1016/j.jct.2010.06.004
Deterpenation of Citrus Essential Oils Using Glycerol-Based Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00944
Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure:	https://www.doi.org/10.1021/je8007414
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Deterpenation of eucalyptus essential oil by liquid + liquid extraction: Phase equilibrium and physical properties for model systems at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2013.09.044
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NIST Webbook:	http://webbook.nist.gov/cbook.cgi?ID=C5989548&Units=SI
Liquid-Liquid Equilibrium for the Water + Acetonitrile + Limonene System at different temperatures:	https://www.doi.org/10.1021/je050066f
Physical Properties of Model and Real Systems Composed of Essential Oils and Hydroalcoholic Solvents at 298.2 K and Atmospheric Pressure:	https://www.doi.org/10.1021/acs.jced.8b00939

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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