Cyclopentane, methyl-

Other names:	Methylcyclopentane
	UN 2298
Inchi:	InChI=1S/C6H12/c1-6-4-2-3-5-6/h6H,2-5H2,1H3
InchiKey:	GDOPTJXRTPNYNR-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CC1CCCC1
Mol. weight [g/mol]:	84.16
CAS:	96-37-7

Physical Properties

Property code	Value	Unit	Source
af	0.2310		KDB
aigt	602.04	K	KDB
ap	306.150	K	KDB
chl	-3938.30 ± 0.59	kJ/mol	NIST Webbook
chl	-3937.70 ± 0.75	kJ/mol	NIST Webbook
chl	-3936.20 ± 1.70	kJ/mol	NIST Webbook
chl	-3956.00	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
fll	1.10	% in Air	KDB
flu	8.70	% in Air	KDB
fpo	255.37	K	KDB
gf	35.80	kJ/mol	KDB
gyrad	3.1670		KDB
hcg	3938.32	kJ/mol	KDB
hcn	3674.263	kJ/mol	KDB
hf	-106.80	kJ/mol	KDB
hf	-108.10	kJ/mol	NIST Webbook
hf	-106.00	kJ/mol	NIST Webbook
hf	-106.70 ± 0.84	kJ/mol	NIST Webbook
hfl	-138.40 ± 0.84	kJ/mol	NIST Webbook
hfl	-137.70 ± 0.71	kJ/mol	NIST Webbook
hfl	-139.80 ± 1.70	kJ/mol	NIST Webbook
hfus	5.23	kJ/mol	Joback Method
hvap	29.21	kJ/mol	Joback Method
ie	9.70 ± 0.10	eV	NIST Webbook
ie	9.85	eV	NIST Webbook

ie	10.34 ± 0.04	eV	NIST Webbook
ie	9.62 ± 0.05	eV	NIST Webbook
ie	10.42	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
log10ws	-3.30		Estimated Solubility Method
log10ws	-3.30		Aqueous Solubility Prediction Method
logp	2.196		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3785.91 ± 5.06	kPa	NIST Webbook
pc	3784.00 ± 40.53	kPa	NIST Webbook
pc	3790.00 ± 40.00	kPa	NIST Webbook
pc	3790.00	kPa	KDB
rhoc	264.26 ± 1.68	kg/m3	NIST Webbook
rhoc	264.01 ± 4.21	kg/m3	NIST Webbook
rhoc	264.26 ± 3.37	kg/m3	NIST Webbook
rinpol	630.80		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	626.60		NIST Webbook
rinpol	628.40		NIST Webbook
rinpol	630.10		NIST Webbook
rinpol	631.50		NIST Webbook
rinpol	638.10		NIST Webbook
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rinpol	625.60	NIST Webbook

rinpol	625.00	NIST Webbook
rinpol	629.00	NIST Webbook
rinpol	623.80	NIST Webbook
rinpol	618.00	NIST Webbook
rinpol	618.70	NIST Webbook
rinpol	627.30	NIST Webbook
rinpol	623.00	NIST Webbook
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rinpol	620.72	NIST Webbook
rinpol	621.00	NIST Webbook
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rinpol	635.00	NIST Webbook

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rinpol	625.40		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	620.72		NIST Webbook
rinpol	628.20		NIST Webbook
ripol	675.00		NIST Webbook
sl	247.78	J/mol×K	NIST Webbook
sl	247.70	J/mol×K	NIST Webbook
tb	344.90	K	KDB
tb	344.96	K	Isobaric Vapor-Liquid Equilibrium Data for Two Binary Systems n-Hexane + 1,2-Dimethoxyethane and Methylcyclopentane + 1,2-Dimethoxyethane at 101.3 kPa
tc	532.70 ± 0.20	K	NIST Webbook
tc	532.70	K	KDB
tc	532.73 ± 0.30	K	NIST Webbook
tc	532.70 ± 0.20	K	NIST Webbook
tc	532.70	K	NIST Webbook
tc	532.76 ± 0.05	K	NIST Webbook
tf	130.65	K	Aqueous Solubility Prediction Method
tf	130.60	K	KDB
vc	0.318	m3/kmol	NIST Webbook
vc	0.318	m3/kmol	KDB
zc	0.2721120		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.21 ± 0.33	J/mol×K	436.25	NIST Webbook
cpg	136.21 ± 0.27	J/mol×K	362.55	NIST Webbook
cpg	124.24 ± 0.25	J/mol×K	333.20	NIST Webbook
cpg	152.15 ± 0.30	J/mol×K	402.35	NIST Webbook
cpg	178.17 ± 0.36	J/mol×K	471.05	NIST Webbook
cpl	157.30	J/mol×K	295.70	NIST Webbook
cpl	157.66	J/mol×K	293.15	NIST Webbook
cpl	159.12	J/mol×K	299.80	NIST Webbook
cpl	158.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0004500	Pa×s	303.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters
dvisc	0.0004760	Pa×s	298.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters

dvisc	0.0005040	Pa×s	293.15	Physical properties of the binary systems methylcyclopentane with ketones (acetone, butanone and 2-pentanone) at T = (293.15, 298.15, and 303.15) K. New UNIFAC-VISCO interaction parameters
dvisc	0.0005040	Pa×s	293.15	Viscosity, density, and speed of sound of methylcyclopentane with primary and secondary alcohols at T = (293.15, 298.15, and 303.15) K
dvisc	0.0004760	Pa×s	298.15	Viscosity, density, and speed of sound of methylcyclopentane with primary and secondary alcohols at T = (293.15, 298.15, and 303.15) K
dvisc	0.0004500	Pa×s	303.15	Viscosity, density, and speed of sound of methylcyclopentane with primary and secondary alcohols at T = (293.15, 298.15, and 303.15) K
hfust	6.93	kJ/mol	130.70	NIST Webbook
hfust	6.93	kJ/mol	130.70	NIST Webbook
hfust	6.88	kJ/mol	130.10	NIST Webbook
hfust	6.93	kJ/mol	130.73	NIST Webbook
hvapt	31.30 ± 0.10	kJ/mol	304.00	NIST Webbook
hvapt	31.40	kJ/mol	322.50	NIST Webbook
hvapt	31.90	kJ/mol	317.00	NIST Webbook
hvapt	30.20 ± 0.10	kJ/mol	326.00	NIST Webbook
hvapt	31.33 ± 0.02	kJ/mol	304.00	NIST Webbook
hvapt	29.08	kJ/mol	345.00	NIST Webbook
hvapt	29.10 ± 0.10	kJ/mol	345.00	NIST Webbook
hvapt	29.08	kJ/mol	345.00	KDB

pvap	101.30	kPa	344.96	Isobaric Vapor-Liquid Equilibrium Data for Two Binary Systems n-Hexane + 1,2-Dimethoxyethane and Methylcyclopentane + 1,2-Dimethoxyethane at 101.3 kPa
rfi	1.40700		298.15	KDB
rfi	1.40670		298.15	Phase equilibria of binary systems of 3-methylthiophene with four different hydrocarbons
rhol	754.00	kg/m3	289.00	KDB
sfust	53.00	J/mol×K	130.73	NIST Webbook
sfust	52.90	J/mol×K	130.10	NIST Webbook
srf	0.02	N/m	293.20	KDB
tcondl	0.12	W/m×K	295.15	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	312.82	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	312.57	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	295.32	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.11	W/m×K	312.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	294.90	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	277.41	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	277.24	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.12	W/m×K	277.00	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	259.11	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	258.96	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	258.71	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42458e+01
Coeff. B	-3.00275e+03

Coeff. C	-3.31070e+01
Temperature range (K), min.	248.23
Temperature range (K), max.	369.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.27581e+01
Coeff. B	-6.08643e+03
Coeff. C	-8.79214e+00
Coeff. D	7.40207e-06
Temperature range (K), min.	130.73
Temperature range (K), max.	532.79

Sources

Partition Coefficients of Organic Compounds in Four New Tetraalkylammonium Bis(trifluoromethylsulfonyl)imide Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je200637v
Phase equilibria of binary systems of 3-methylthiophene with four different ketones (acetone, butanone and 2-pentanone) at 293.15, 298.15, and 303.15 K:	https://www.doi.org/10.1016/j.fluid.2009.11.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Physical properties of the binary systems methylcyclopentane with 1,2-dimethoxyethane at 101.18 kPa:	https://www.doi.org/10.1016/j.jct.2005.08.002
Activity coefficients at infinite dilution of organic solutes in 2-pentanone and 2-methoxyethanol at 298.15 K:	https://www.doi.org/10.1016/j.jct.2015.02.023
Liquid-liquid equilibria for the binary systems of N-formylmorpholine with alkanes and cycloalkanes:	https://www.doi.org/10.1021/je020208v
Validation Parameters:	https://www.cheric.org/files/research/kdb/mol/mol469.mol
Liquid liquid equilibria for the binary systems of sulfolane with branched cycloalkanes:	https://www.doi.org/10.1016/j.fluid.2006.05.008
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Isobaric Vapor-Liquid Equilibrium Data for Two Binary Systems n-Hexane + 1,2-Dimethoxyethane and Methylcyclopentane + 1,2-Dimethoxyethane at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.7b00802
Infinite Dilution Activity Coefficients of Solutes Dissolved in Two Ether-Functionalized Ionic Liquids:	https://www.doi.org/10.1021/je500050p
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Study of Ether-, Alcohol-, or Cyano-Functionalized Ionic Liquids:	https://www.doi.org/10.1021/je034162x
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Thermodynamics of solvation in propylene glycol and methyl cellosolve:	https://www.doi.org/10.1016/j.jct.2014.06.006
Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Activity Coefficients at Infinite Dilution of Organic Compounds in 1-Butyl-3-methylimidazolium Tetrafluoroborate Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je800658v

Viscosity, density, and speed of sound of methylcyclopentane with primary and secondary alcohols at T = (293.15, 298.15, and 303.15) K:	https://www.doi.org/10.1016/j.jct.2005.12.010
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=469
Activity Coefficients at Infinite Dilution of Organic Compounds in Four New Imidazolium Based Ionic Liquids:	https://www.doi.org/10.1021/je200195q
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96377&Units=SI
Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2010.02.030
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Activity Coefficients at Infinite Dilution for Organic Solutes Dissolved in Three Ionic Liquids Having Common Bis(trifluoromethylsulfonyl)imide Ionic Liquids Bearing Short Linear Alkyl Side Chains of Three to Five Carbons:	https://www.doi.org/10.1021/je4001894
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure

rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter