

# Cycloheptane

**Inchi:** InChI=1S/C7H14/c1-2-4-6-7-5-3-1/h1-7H2  
**InchiKey:** DMEGYFMYUHOHGS-UHFFFAOYSA-N  
**Formula:** C7H14  
**SMILES:** C1CCCCC1  
**Mol. weight [g/mol]:** 98.19  
**CAS:** 291-64-5

## Physical Properties

Property code	Value	Unit	Source
af	0.2370		KDB
chl	-4597.60 ± 0.60	kJ/mol	NIST Webbook
chl	-4598.90 ± 1.70	kJ/mol	NIST Webbook
chl	-4586.50	kJ/mol	NIST Webbook
chl	-4597.00 ± 0.80	kJ/mol	NIST Webbook
gf	63.05	kJ/mol	KDB
hcg	4597.80	kJ/mol	KDB
hcn	4289.856	kJ/mol	KDB
hf	-119.40	kJ/mol	KDB
hfl	-156.40 ± 1.70	kJ/mol	NIST Webbook
hfus	2.55	kJ/mol	Joback Method
hvap	38.50 ± 0.20	kJ/mol	NIST Webbook
hvap	39.40	kJ/mol	NIST Webbook
hvap	38.50	kJ/mol	NIST Webbook
hvap	38.50 ± 2.10	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
ie	9.97	eV	NIST Webbook
ie	9.96	eV	NIST Webbook
ie	9.82 ± 0.05	eV	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	9.88 ± 0.05	eV	NIST Webbook
log10ws	-3.51		Estimated Solubility Method
log10ws	-3.52		Aqueous Solubility Prediction Method
logp	2.731		Crippen Method
mcpvol	98.630	ml/mol	McGowan Method
pc	3820.00	kPa	KDB
pc	3820.00 ± 40.00	kPa	NIST Webbook

pc	3813.00 ± 50.00	kPa	NIST Webbook
pc	3826.00 ± 40.53	kPa	NIST Webbook
rhoc	277.87 ± 3.93	kg/m3	NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	811.60		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	795.00		NIST Webbook
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rinpol	794.00		NIST Webbook
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rinpol	800.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	803.00		NIST Webbook
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rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	837.50		NIST Webbook
rinpol	806.90		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	800.00		NIST Webbook

rinpol	819.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	806.90		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	794.20		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	837.50		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	789.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	892.00		NIST Webbook
sg	342.30 ± 1.30	J/mol×K	NIST Webbook
sl	242.55	J/mol×K	NIST Webbook
tb	392.15 ± 2.00	K	NIST Webbook
tb	391.25 ± 0.60	K	NIST Webbook
tb	391.63	K	KDB
tb	391.70	K	NIST Webbook
tb	393.00 ± 2.00	K	NIST Webbook
tb	391.63 ± 0.30	K	NIST Webbook
tb	391.99 ± 0.30	K	NIST Webbook
tb	391.99 ± 0.30	K	NIST Webbook
tb	391.99 ± 0.20	K	NIST Webbook
tc	604.20	K	KDB
tc	604.20 ± 0.50	K	NIST Webbook
tc	604.20 ± 0.50	K	NIST Webbook
tf	265.12	K	KDB
tt	265.00 ± 0.07	K	NIST Webbook
tt	265.12 ± 0.05	K	NIST Webbook
tt	265.10 ± 3.00	K	NIST Webbook
vc	0.353	m3/kmol	KDB
vc	0.354 ± 0.007	m3/kmol	NIST Webbook
vc	0.353	m3/kmol	NIST Webbook
zc	0.2684240		KDB

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.82	J/molxK	423.39	Joback Method
cpg	170.69	J/molxK	388.05	Joback Method
cpg	260.93	J/molxK	600.09	Joback Method
cpg	247.91	J/molxK	564.75	Joback Method
cpg	234.11	J/molxK	529.41	Joback Method
cpg	219.50	J/molxK	494.07	Joback Method
cpg	204.08	J/molxK	458.73	Joback Method
cpl	180.75	J/molxK	298.15	NIST Webbook
cpl	180.47	J/molxK	298.15	NIST Webbook
cpl	180.61	J/molxK	298.15	NIST Webbook
dvisc	0.0332403	Paxs	176.75	Joback Method
dvisc	0.0006718	Paxs	317.62	Joback Method
dvisc	0.0012369	Paxs	282.40	Joback Method
dvisc	0.0027104	Paxs	247.18	Joback Method
dvisc	0.0004121	Paxs	352.83	Joback Method
dvisc	0.0077075	Paxs	211.97	Joback Method
dvisc	0.0002763	Paxs	388.05	Joback Method
hfust	0.29	kJ/mol	198.20	NIST Webbook
hfust	4.98	kJ/mol	134.80	NIST Webbook
hfust	1.88	kJ/mol	265.10	NIST Webbook
hfust	0.45	kJ/mol	212.40	NIST Webbook
hfust	1.88	kJ/mol	265.10	NIST Webbook
hsubt	53.50	kJ/mol	134.00	NIST Webbook
hvapt	36.40	kJ/mol	365.50	NIST Webbook
hvapt	31.70	kJ/mol	540.00	NIST Webbook
hvapt	36.10	kJ/mol	387.00	NIST Webbook
hvapt	38.60	kJ/mol	307.50	NIST Webbook
rfi	1.44240		298.15	KDB
rhoI	810.00	kg/m3	293.00	KDB
sfust	7.10	J/molxK	265.10	NIST Webbook
sfust	2.11	J/molxK	212.40	NIST Webbook
sfust	1.46	J/molxK	198.20	NIST Webbook
sfust	36.94	J/molxK	134.80	NIST Webbook
srf	0.03	N/m	298.20	KDB

tcondl	0.11	W/m×K	320.05	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.01	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	280.48	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	280.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	262.50	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	262.37	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	262.18	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.20	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.33	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	320.23	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.11	W/m×K	320.36	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	280.35	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41291e+01
Coeff. B	-3.26491e+03
Coeff. C	-4.86550e+01
Temperature range (K), min.	265.12
Temperature range (K), max.	418.93

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.37466e+01
Coeff. B	-7.38221e+03
Coeff. C	-1.02752e+01
Coeff. D	6.91167e-06
Temperature range (K), min.	265.12
Temperature range (K), max.	604.30

# Sources

Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from river basins as a function of dilution and physicochemical properties of organic solutes in water. The ionic liquid (2-methoxyethyl)-

1-methyl-3-methylimidazolium (2-methoxy-ethyl)ammonium

for separation of organic solutes from river basins

Separation of Various Solutes in

Tetrahydrofuran-Bromine

for Separation of Deep Eutectic Solvent:

Tris(hydroxymethyl)aminomethane:

bis(trifluoromethylsulfonyl)imide ionic liquid using gas liquid

chromatography.

Activity Coefficients at Infinite Dilution

of Organic Compounds in Four New

Therapeutic Based on Molecular

Interaction-selectivity in separation

processes based on limiting activity

and physicochemical properties for

organic solutes and separation of ionic

separation based on activity

for organic compounds dissolved in:

Activity Coefficients at Infinite Dilution

for Organic Compounds Dissolved in:

Activity Coefficients at Infinite Dilution

for Organic Compounds Dissolved in:

Activity Coefficients at Infinite Dilution

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Activity Coefficients at Infinite Dilution

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<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>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rfi:</b>	Refractive Index
<b>rhoc:</b>	Critical density
<b>rhof:</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>sg:</b>	Molar entropy at standard conditions
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tcondl:</b>	Liquid thermal conductivity
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume
<b>zc:</b>	Critical Compressibility

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