

# 1,3-Cyclohexadiene

<b>Other names:</b>	1,2-Dihydrobenzene Cyclohexa-1,3-diene
<b>Inchi:</b>	InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-4H,5-6H2
<b>InchiKey:</b>	MGNZXYWBUKAI-UHFFFAOYSA-N
<b>Formula:</b>	C6H8
<b>SMILES:</b>	C1=CCCC=C1
<b>Mol. weight [g/mol]:</b>	80.13
<b>CAS:</b>	592-57-4

## Physical Properties

Property code	Value	Unit	Source
affp	837.00	kJ/mol	NIST Webbook
basg	804.50	kJ/mol	NIST Webbook
chl	-3575.79 ± 0.54	kJ/mol	NIST Webbook
gf	91.72	kJ/mol	Joback Method
hf	104.58 ± 0.63	kJ/mol	NIST Webbook
hfl	71.41 ± 0.62	kJ/mol	NIST Webbook
hfus	4.50	kJ/mol	Joback Method
hvap	33.17 ± 0.05	kJ/mol	NIST Webbook
hvap	33.20	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
ie	8.25 ± 0.02	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
ie	8.28 ± 0.05	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.25 ± 0.03	eV	NIST Webbook
ie	8.25 ± 0.03	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.893		Crippen Method
mvol	75.940	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	665.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	653.00		NIST Webbook

rinpol	655.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	653.40		NIST Webbook
rinpol	652.80		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	673.10		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	688.60		NIST Webbook
rinpol	689.60		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	665.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	861.00		NIST Webbook
ripol	861.00		NIST Webbook
sl	197.28	J/molxK	NIST Webbook
tb	359.22	K	Joback Method
tc	568.24	K	Joback Method
tf	168.40 ± 0.30	K	NIST Webbook
tf	184.00 ± 4.00	K	NIST Webbook
tt	161.00 ± 0.20	K	NIST Webbook
vc	0.278	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.19	J/molxK	463.73	Joback Method
cpg	124.27	J/molxK	394.06	Joback Method
cpg	112.28	J/molxK	359.22	Joback Method
cpg	156.16	J/molxK	498.57	Joback Method
cpg	165.52	J/molxK	533.40	Joback Method
cpg	174.29	J/molxK	568.24	Joback Method
cpg	135.57	J/molxK	428.89	Joback Method
cpl	141.30	J/molxK	298.15	NIST Webbook
cpl	144.56	J/molxK	298.15	NIST Webbook
dvisc	0.0004717	Paxs	296.32	Joback Method
dvisc	0.0007201	Paxs	264.87	Joback Method
dvisc	0.0002528	Paxs	359.22	Joback Method
dvisc	0.0024921	Paxs	201.97	Joback Method
dvisc	0.0065358	Paxs	170.52	Joback Method
dvisc	0.0003351	Paxs	327.77	Joback Method
dvisc	0.0012321	Paxs	233.42	Joback Method
hfust	4.20	kJ/mol	161.00	NIST Webbook
hfust	4.20	kJ/mol	161.00	NIST Webbook
hfust	4.20	kJ/mol	161.00	NIST Webbook
hvapt	32.60	kJ/mol	335.50	NIST Webbook
hvapt	32.40	kJ/mol	313.00	NIST Webbook
sfust	26.11	J/molxK	161.00	NIST Webbook
tcondl	0.12	W/mxK	329.08	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/mxK	328.84	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	328.56	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	314.41	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	314.22	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	313.95	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	296.69	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	296.51	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	296.25	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	279.41	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	279.31	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	279.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.14	W/m×K	264.89	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	264.80	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	264.66	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	258.62	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	258.52	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl

0.15

W/m×K

258.35

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	$\ln(P_{\text{vp}}) = A + B/(T + C)$
Coeff. A	1.43947e+01
Coeff. B	-3.11805e+03
Coeff. C	-3.50620e+01
Temperature range (K), min.	256.09
Temperature range (K), max.	378.34

## Sources

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- 1-Methyl-3-octyl-imidazolium Tetrafluoroborate Using Gas-Liquid Chromatography:  
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<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

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