

# Cyclohexane-d12

<b>Other names:</b>	( <sup>2</sup> H <sub>12</sub> )cyclohexane [2H12]cyclohexane cyclohexane-2H12 perdeuterated cyclohexane perdeuteriocyclohexane
<b>Inchi:</b>	InChI=1S/C6H12/c1-2-4-6-5-3-1/h1-6H2/i1D2,2D2,3D2,4D2,5D2,6D2
<b>InchiKey:</b>	XDTMQSROBMDMFD-LBTWDOQPSA-N
<b>Formula:</b>	C6D12
<b>SMILES:</b>	C1CCCCC1
<b>Mol. weight [g/mol]:</b>	96.23
<b>CAS:</b>	1735-17-7

## Physical Properties

Property code	Value	Unit	Source
gf	31.80	kJ/mol	Joback Method
hf	-92.51	kJ/mol	Joback Method
hfus	2.06	kJ/mol	Joback Method
hvap	33.10	kJ/mol	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	9.91 ± 0.01	eV	NIST Webbook
ie	9.93 ± 0.15	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
log10ws	-2.23		Crippen Method
logp	2.341		Crippen Method
mvol	84.540	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	661.00		NIST Webbook
sl	228.20	J/mol×K	NIST Webbook
tb	360.90	K	Joback Method
tc	565.41	K	Joback Method
tf	169.00	K	Joback Method
vc	0.305	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.03	J/mol×K	360.90	Joback Method
cpg	162.77	J/mol×K	429.07	Joback Method
cpg	176.04	J/mol×K	463.15	Joback Method
cpg	188.60	J/mol×K	497.24	Joback Method
cpg	200.49	J/mol×K	531.32	Joback Method
cpg	211.71	J/mol×K	565.41	Joback Method
cpg	148.78	J/mol×K	394.98	Joback Method
cpl	188.70	J/mol×K	298.15	NIST Webbook
cpl	183.84	J/mol×K	298.00	NIST Webbook
dvisc	0.0153533	Paxs	169.00	Joback Method
dvisc	0.0047435	Paxs	200.98	Joback Method
dvisc	0.0020233	Paxs	232.97	Joback Method
dvisc	0.0010601	Paxs	264.95	Joback Method
dvisc	0.0006385	Paxs	296.93	Joback Method
dvisc	0.0004244	Paxs	328.92	Joback Method
dvisc	0.0003032	Paxs	360.90	Joback Method
hvapt	32.58	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
tcondl	0.11	W/m×K	303.67	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.10	W/m×K	326.30	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.11	W/m×K	316.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	316.06	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	315.91	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	303.92	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	303.83	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.10	W/m×K	326.44	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	291.45	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	291.34	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	291.18	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	280.74	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	280.63	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	280.46	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.10	W/m×K	326.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

## Sources

Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons: Joback Method  
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<https://www.doi.org/10.1021/je800091s>

Deuterium isotope effects in liquid phase diagrams of aniline + trihexyl(tetradecyl)phosphonium hexafluorophosphate with cyclic hydrocarbons: McGowan Method:

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Miscibility behavior of trihexyl(tetradecyl)phosphonium hexafluorophosphate with cyclic hydrocarbons: McGowan Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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<http://link.springer.com/article/10.1007/BF02311772>

Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<https://www.doi.org/10.1021/je034162x>

# Legend

<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>hfus:</b>	Enthalpy of fusion at standard conditions
<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>rinpol:</b>	Non-polar retention indices
<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>vc:</b>	Critical Volume

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