1,4-Cyclohexadiene

Other names: 1,4-Dihydrobenzene
Cyclohexa-1,4-diene
Inchi: InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-2,5-6H,3-4H2
InchiKey: UVJHQYIOXKWHFD-UHFFFAOYSA-N
Formula: C6H8
SMILES: C1=CCC=CC1
Mol. weight [g/mol]: 80.13
CAS: 628-41-1

Physical Properties

Property code	Value	Unit	Source
affp	837.00	kJ/mol	NIST Webbook
basg	808.00	kJ/mol	NIST Webbook
chl	-3570.50 ± 3.00	kJ/mol	NIST Webbook
chl	-3574.08 ± 0.48	kJ/mol	NIST Webbook
gf	91.72	kJ/mol	Joback Method
hf	104.75 ± 0.59	kJ/mol	NIST Webbook
hf	109.00	kJ/mol	NIST Webbook
hf	100.40 ± 3.10	kJ/mol	NIST Webbook
hfl	69.70 ± 0.58	kJ/mol	NIST Webbook
hfl	66.10 ± 3.10	kJ/mol	NIST Webbook
hfus	4.50	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
hvap	35.05 ± 0.04	kJ/mol	NIST Webbook
hvap	34.30	kJ/mol	NIST Webbook
hvap	35.10	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.65 ± 0.05	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-2.06		Estimated Solubility Method

log10ws	-1.97		Aqueous Solubility Prediction Method
logp	1.893		Crippen Method
mcvol	75.940	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	694.00		NIST Webbook
rinpol	724.90		NIST Webbook
rinpol	709.20		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	725.30		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	708.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	914.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	939.00		NIST Webbook
sl	189.37	J/mol×K	NIST Webbook
tb	362.70 ± 0.20	K	NIST Webbook
tb	362.55 ± 0.30	K	NIST Webbook

tb	354.70	K	NIST Webbook
tc	568.24	K	Joback Method
tf	351.00 ± 4.00	K	NIST Webbook
tf	224.05	K	Aqueous Solubility Prediction Method
tf	222.83 ± 0.20	K	NIST Webbook
tt	224.00 ± 0.20	K	NIST Webbook
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.29	J/mol×K	568.24	Joback Method
cpg	124.27	J/mol×K	394.06	Joback Method
cpg	165.52	J/mol×K	533.40	Joback Method
cpg	156.16	J/mol×K	498.57	Joback Method
cpg	146.19	J/mol×K	463.73	Joback Method
cpg	135.57	J/mol×K	428.89	Joback Method
cpg	112.28	J/mol×K	359.22	Joback Method
cpl	142.20	J/mol×K	298.15	NIST Webbook
cpl	145.94	J/mol×K	298.15	NIST Webbook
dvisc	0.0002528	Pa×s	359.22	Joback Method
dvisc	0.0065358	Pa×s	170.52	Joback Method
dvisc	0.0012321	Pa×s	233.42	Joback Method
dvisc	0.0007201	Pa×s	264.87	Joback Method
dvisc	0.0004717	Pa×s	296.32	Joback Method
dvisc	0.0003351	Pa×s	327.77	Joback Method
dvisc	0.0024921	Pa×s	201.97	Joback Method
hfust	5.72	kJ/mol	224.00	NIST Webbook
hfust	0.82	kJ/mol	192.00	NIST Webbook
hfust	5.72	kJ/mol	224.00	NIST Webbook
hvapt	33.90	kJ/mol	313.00	NIST Webbook
hvapt	34.00	kJ/mol	332.00	NIST Webbook
sfust	4.25	J/mol×K	192.00	NIST Webbook
sfust	25.51	J/mol×K	224.00	NIST Webbook

tcondl	0.16	W/m×K	258.46	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	279.76	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	296.20	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	296.43	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	296.60	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.14	W/m×K	313.90	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	314.13	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	314.31	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	328.51	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	328.75	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	328.93	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	279.60	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	279.38	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.16	W/m×K	265.23	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.16	W/m×K	264.86	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.16	W/m×K	258.82	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.16	W/m×K	258.67	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.16	W/m×K	265.08	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	1.42725e+01
Coeff. B	-2.23809e+03
Coeff. C	-1.16823e+02
Temperature range (K), min.	276.86
Temperature range (K), max.	366.58

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic Alkanes, Alkenes, Alkynes, Aromatics), and Deuterated Hydrocarbons:	https://www.doi.org/10.1021/je034162x
Infinite dilution activity coefficients, specific retention volumes and Abraham model correlations for hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
NIST WebBook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628411&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
pvap:	Vapor pressure
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume