Cyclopentene

Inchi: InChI=1S/C5H8/c1-2-4-5-3-1/h1-2H,3-5H2
InchiKey: LPIQUOYDBNQMRZ-UHFFFAOYSA-N
Formula: C5H8
SMILES: C1=CCCC1
Mol. weight [g/mol]: 68.12
CAS: 142-29-0

Physical Properties

Property code	Value	Unit	Source
af	0.2060		KDB
affp	766.30	kJ/mol	NIST Webbook
ap	263.150	K	KDB
basg	733.80	kJ/mol	NIST Webbook
chl	-3115.20 ± 0.59	kJ/mol	NIST Webbook
dm	0.90	debye	KDB
gf	190.90	kJ/mol	KDB
hcg	3115.20	kJ/mol	KDB
hcn	2939.134	kJ/mol	KDB
hf	33.20	kJ/mol	NIST Webbook
hf	32.95	kJ/mol	KDB
hf	32.60	kJ/mol	NIST Webbook
hf	34.00	kJ/mol	NIST Webbook
hf	36.00	kJ/mol	NIST Webbook
hfl	4.27 ± 0.63	kJ/mol	NIST Webbook
hfl	4.85 ± 0.67	kJ/mol	NIST Webbook
hfus	2.79	kJ/mol	Joback Method
hvap	28.37	kJ/mol	NIST Webbook
ie	9.02 ± 0.01	eV	NIST Webbook
ie	9.01 ± 0.03	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.01	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook

ie	9.02 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	9.01 ± 0.02	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.10		Aqueous Solubility Prediction Method
log10ws	-2.10		Estimated Solubility Method
logp	1.727		Crippen Method
mcvol	66.150	ml/mol	McGowan Method
pc	4802.00 ± 30.00	kPa	NIST Webbook
pc	4800.00 ± 50.00	kPa	NIST Webbook
pc	4800.00	kPa	KDB
rhoc	277.92 ± 6.13	kg/m3	NIST Webbook
rhoc	277.92 ± 3.41	kg/m3	NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	549.50		NIST Webbook
rinpol	551.40		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	547.00		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	549.62		NIST Webbook
rinpol	548.20		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	557.90		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	572.00		NIST Webbook
rinpol	545.48		NIST Webbook
rinpol	561.80		NIST Webbook
rinpol	549.60		NIST Webbook
rinpol	550.70		NIST Webbook
rinpol	555.50		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.30		NIST Webbook

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rinpol	561.00	NIST Webbook
rinpol	566.50	NIST Webbook
rinpol	562.00	NIST Webbook
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rinpol	549.50	NIST Webbook

rinpol	549.62		NIST Webbook
rinpol	552.00		NIST Webbook
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rinpol	550.10		NIST Webbook
rinpol	557.00		NIST Webbook
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rinpol	550.00		NIST Webbook
rinpol	566.50		NIST Webbook
rinpol	569.50		NIST Webbook
rinpol	547.70		NIST Webbook
rinpol	562.30		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	561.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	547.00		NIST Webbook
ripol	663.00		NIST Webbook
ripol	693.30		NIST Webbook
ripol	704.90		NIST Webbook
ripol	663.00		NIST Webbook
ripol	693.30		NIST Webbook
ripol	705.00		NIST Webbook
ripol	705.00		NIST Webbook
ripol	701.00		NIST Webbook
ripol	693.00		NIST Webbook
ripol	700.70		NIST Webbook
ripol	700.70		NIST Webbook
ripol	693.30		NIST Webbook
ripol	705.00		NIST Webbook
ripol	704.40		NIST Webbook
sg	289.66	J/mol×K	NIST Webbook
sl	201.25	J/mol×K	NIST Webbook
tb	317.55 ± 0.20	K	NIST Webbook
tb	315.00 ± 3.00	K	NIST Webbook

tb	317.00 ± 1.50	K	NIST Webbook
tb	317.50 ± 1.00	K	NIST Webbook
tb	317.40 ± 0.40	K	NIST Webbook
tb	317.00 ± 2.00	K	NIST Webbook
tb	317.30 ± 1.00	K	NIST Webbook
tb	317.60 ± 1.50	K	NIST Webbook
tb	317.00 ± 2.00	K	NIST Webbook
tb	317.55 ± 0.25	K	NIST Webbook
tb	317.38 ± 0.20	K	NIST Webbook
tb	317.40 ± 0.20	K	NIST Webbook
tb	316.00 ± 3.00	K	NIST Webbook
tb	317.50 ± 0.50	K	NIST Webbook
tb	317.50 ± 0.50	K	NIST Webbook
tb	318.12 ± 0.02	K	NIST Webbook
tb	316.90 ± 0.60	K	NIST Webbook
tb	319.00 ± 2.00	K	NIST Webbook
tb	319.00 ± 2.00	K	NIST Webbook
tb	317.17 ± 0.20	K	NIST Webbook
tb	317.00 ± 1.00	K	NIST Webbook
tb	317.40	K	NIST Webbook
tb	317.39	K	KDB
tb	317.40 ± 2.00	K	NIST Webbook
tb	320.00 ± 4.00	K	NIST Webbook
tb	317.30 ± 1.50	K	NIST Webbook
tb	317.00 ± 4.00	K	NIST Webbook
tb	317.39 ± 0.10	K	NIST Webbook
tb	316.00 ± 5.00	K	NIST Webbook
tc	506.50	K	KDB
tc	506.10 ± 0.15	K	NIST Webbook
tc	507.60 ± 0.40	K	NIST Webbook
tc	506.50 ± 0.50	K	NIST Webbook
tc	507.00 ± 0.60	K	NIST Webbook
tf	138.00	K	KDB
tf	138.12	K	Aqueous Solubility Prediction Method
tt	138.13 ± 0.05	K	NIST Webbook
vc	0.245	m3/kmol	NIST Webbook
vc	0.245	m3/kmol	KDB
zc	0.2792490		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.35	J/mol×K	432.09	Joback Method
cpg	112.57	J/mol×K	399.03	Joback Method
cpg	148.33	J/mol×K	531.28	Joback Method
cpg	140.20	J/mol×K	498.22	Joback Method
cpg	131.55	J/mol×K	465.15	Joback Method
cpg	91.20	J/mol×K	332.91	Joback Method
cpg	102.20	J/mol×K	365.97	Joback Method
cpl	122.38	J/mol×K	298.15	NIST Webbook
dvisc	0.0004439	Pa×s	275.94	Joback Method
dvisc	0.0009838	Pa×s	218.98	Joback Method
dvisc	0.0003334	Pa×s	304.43	Joback Method
dvisc	0.0002630	Pa×s	332.91	Joback Method
dvisc	0.0038152	Pa×s	162.01	Joback Method
dvisc	0.0017506	Pa×s	190.49	Joback Method
dvisc	0.0006312	Pa×s	247.46	Joback Method
hfust	3.36	kJ/mol	138.10	NIST Webbook
hfust	0.48	kJ/mol	87.07	NIST Webbook
hfust	3.36	kJ/mol	138.10	NIST Webbook
hvapt	26.99	kJ/mol	317.40	KDB
hvapt	29.90	kJ/mol	283.50	NIST Webbook
hvapt	24.80	kJ/mol	303.50	NIST Webbook
hvapt	28.40	kJ/mol	261.50	NIST Webbook
rfi	1.41940		298.15	KDB
rfi	1.42240		293.15	Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa
rhol	772.00	kg/m3	293.00	KDB
sfust	24.32	J/mol×K	138.10	NIST Webbook
sfust	5.51	J/mol×K	87.07	NIST Webbook
srf	0.02	N/m	293.20	KDB
tcondl	0.15	W/m×K	259.10	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.14	W/m×K	276.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.14	W/m×K	277.23	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.14	W/m×K	277.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.15	W/m×K	258.94	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	295.16	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	295.33	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	312.58	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	312.84	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	313.02	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.15	W/m×K	258.72	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	294.92	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	1.43557e+01
Coeff. B	-2.79261e+03
Coeff. C	-3.02070e+01
Temperature range (K), min.	228.71
Temperature range (K), max.	338.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.73094e+01
Coeff. B	-5.41966e+03
Coeff. C	-8.05798e+00
Coeff. D	7.94719e-06
Temperature range (K), min.	138.13
Temperature range (K), max.	507.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol609.mol
Relation between characteristic molecular volume and hydrophobicity of nonpolar molecules:	https://www.doi.org/10.1016/j.jct.2010.04.011
Isobaric Vapor-Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa:	https://www.doi.org/10.1021/acs.jced.6b00180
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=609
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons.:	https://www.doi.org/10.1021/je034162x
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Systems with ionic liquids: Measurement of VLE and c1 data and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(Ol):	https://www.doi.org/10.1016/j.jct.2005.04.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
affp:	Proton affinity
ap:	Aniline Point
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
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

sg:	Molar entropy at standard conditions
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
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility