

Cyclopentane, ethyl-

Other names:	Ethylcyclopentane
Inchi:	InChI=1S/C7H14/c1-2-7-5-3-4-6-7/h7H,2-6H2,1H3
InchiKey:	IFTRQJLVEBNKJK-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCC1CCCC1
Mol. weight [g/mol]:	98.19
CAS:	1640-89-7

Physical Properties

Property code	Value	Unit	Source
af	0.2710		KDB
ap	309.850	K	KDB
chl	-4591.94 ± 0.92	kJ/mol	NIST Webbook
chl	-4589.60 ± 1.50	kJ/mol	NIST Webbook
gf	44.59	kJ/mol	KDB
hcg	4591.94	kJ/mol	KDB
hcn	4283.872	kJ/mol	KDB
hf	-129.40	kJ/mol	NIST Webbook
hf	-127.20	kJ/mol	KDB
hf	-127.10 ± 1.00	kJ/mol	NIST Webbook
hfl	-165.80 ± 1.60	kJ/mol	NIST Webbook
hfl	-163.50 ± 1.00	kJ/mol	NIST Webbook
hfus	7.82	kJ/mol	Joback Method
hvap	36.50	kJ/mol	NIST Webbook
hvap	36.40	kJ/mol	NIST Webbook
hvap	36.47	kJ/mol	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	10.12 ± 0.02	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.587		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3397.02 ± 5.06	kPa	NIST Webbook
pc	3400.00 ± 40.00	kPa	NIST Webbook
pc	3400.00	kPa	KDB
rhoc	262.16 ± 1.96	kg/m3	NIST Webbook

rhoc	262.16 ± 3.93	kg/m3	NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	734.30		NIST Webbook
rinpol	734.80		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
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ripol	809.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	817.00		NIST Webbook
ripol	773.00		NIST Webbook
sg	378.32	J/mol×K	NIST Webbook
sl	279.91	J/mol×K	NIST Webbook
tb	376.60	K	KDB
tc	569.45 ± 0.05	K	NIST Webbook
tc	569.50	K	NIST Webbook
tc	569.50 ± 0.50	K	NIST Webbook
tc	569.50	K	KDB
tf	134.71	K	KDB
vc	0.375	m3/kmol	KDB
vc	0.375	m3/kmol	NIST Webbook
zc	0.2692650		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.21	J/mol×K	568.84	Joback Method
cpg	243.33	J/mol×K	536.50	Joback Method
cpg	173.92	J/mol×K	374.84	Joback Method
cpg	189.22	J/mol×K	407.17	Joback Method
cpg	203.78	J/mol×K	439.51	Joback Method
cpg	217.64	J/mol×K	471.84	Joback Method
cpg	230.81	J/mol×K	504.17	Joback Method
cpl	187.61	J/mol×K	301.83	NIST Webbook
dvisc	0.0002960	Pa×s	374.84	Joback Method
dvisc	0.0004849	Pa×s	309.74	Joback Method
dvisc	0.0038089	Pa×s	179.55	Joback Method
dvisc	0.0017947	Pa×s	212.10	Joback Method
dvisc	0.0010331	Pa×s	244.65	Joback Method

dvisc	0.0006770	Pa×s	277.19	Joback Method
dvisc	0.0003701	Pa×s	342.29	Joback Method
hfust	6.87	kJ/mol	134.70	NIST Webbook
hfust	6.86	kJ/mol	134.70	NIST Webbook
hvapt	35.70	kJ/mol	339.50	NIST Webbook
hvapt	32.50 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	33.00 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	32.28	kJ/mol	376.60	KDB
hvapt	31.96	kJ/mol	376.60	NIST Webbook
hvapt	35.50	kJ/mol	347.50	NIST Webbook
hvapt	32.90	kJ/mol	446.50	NIST Webbook
hvapt	31.90	kJ/mol	534.00	NIST Webbook
hvapt	35.60 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	34.80 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	33.90 ± 0.10	kJ/mol	343.00	NIST Webbook
rfi	1.41730		298.15	KDB
rhoI	771.00	kg/m3	289.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43149e+01
Coeff. B	-3.29180e+03
Coeff. C	-3.71200e+01
Temperature range (K), min.	271.79
Temperature range (K), max.	402.74

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.15619e+01
Coeff. B	-7.00763e+03
Coeff. C	-1.00117e+01
Coeff. D	7.36714e-06
Temperature range (K), min.	134.71
Temperature range (K), max.	569.52

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1640897&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=471
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol471.mol

Legend

af:	Acentric Factor
ap:	Aniline Point
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index

rhoc:	Critical density
rhoL:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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