Cyclopentane, 1-ethyl-1-methyl-

Other names:	1-ETHYL-1-METHYLCYCLOPENTANE
	1-Methyl-1-ethylcyclopentane
Inchi:	InChI=1S/C8H16/c1-3-8(2)6-4-5-7-8/h3-7H2,1-2H3
InchiKey:	LETYIFNDQBJGPJ-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CCC1(C)CCCC1
Mol. weight [g/mol]:	112.21
CAS:	16747-50-5

Physical Properties

Property code	Value	Unit	Source
af	0.2500		KDB
chl	-5240.96 ± 0.92	kJ/mol	NIST Webbook
gf	47.54	kJ/mol	Joback Method
hcg	5242.55	kJ/mol	KDB
hcn	4890.260	kJ/mol	KDB
hf	-132.73	kJ/mol	Joback Method
hfl	-193.80 ± 1.00	kJ/mol	NIST Webbook
hfus	4.11	kJ/mol	Joback Method
hvap	38.80	kJ/mol	NIST Webbook
hvap	38.90	kJ/mol	NIST Webbook
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.977		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3000.00	kPa	KDB
rinpol	793.00		NIST Webbook
rinpol	796.10		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	796.10		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	793.00		NIST Webbook

rinpol	793.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	788.80	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	792.80	NIST Webbook
rinpol	785.82	NIST Webbook
rinpol	786.23	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	794.60	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	793.40	NIST Webbook
rinpol	794.90	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	798.70	NIST Webbook
rinpol	800.10	NIST Webbook
rinpol	801.40	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	801.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	794.30	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	794.30	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	797.90	NIST Webbook
rinpol	793.10	NIST Webbook
rinpol	805.00	NIST Webbook

rinpol	805.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	799.00		NIST Webbook
tb	394.70	K	NIST Webbook
tb	394.70	K	KDB
tb	394.67 ± 0.20	K	NIST Webbook
tb	395.00 ± 3.00	K	NIST Webbook
tb	394.65 ± 0.50	K	NIST Webbook
tb	394.67 ± 0.02	K	NIST Webbook
tb	394.60 ± 0.15	K	NIST Webbook
tb	394.65 ± 0.40	K	NIST Webbook
tc	592.00	K	KDB
tc	592.00	K	NIST Webbook
tf	129.35 ± 0.10	K	NIST Webbook
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.33 ± 0.52	J/mol×K	498.15	NIST Webbook
cpg	202.60 ± 0.41	J/mol×K	383.15	NIST Webbook
cpg	210.66 ± 0.42	J/mol×K	398.15	NIST Webbook
cpg	223.08 ± 0.45	J/mol×K	423.15	NIST Webbook
cpg	235.59 ± 0.47	J/mol×K	448.15	NIST Webbook
cpg	247.63 ± 0.50	J/mol×K	473.15	NIST Webbook
cpg	270.33 ± 0.54	J/mol×K	523.15	NIST Webbook
hvapt	33.20	kJ/mol	394.70	NIST Webbook
hvapt	36.70	kJ/mol	364.00	NIST Webbook
hvapt	40.20	kJ/mol	263.00	NIST Webbook
hvapt	37.30	kJ/mol	356.00	NIST Webbook
rfi	1.42476		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45909e+01

Coeff. B	-3.62175e+03
Coeff. C	-3.15290e+01
Temperature range (K), min.	284.74
Temperature range (K), max.	421.83

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.43448e+01
Coeff. B	-7.03824e+03
Coeff. C	-8.81550e+00
Coeff. D	5.18879e-06
Temperature range (K), min.	238.15
Temperature range (K), max.	592.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol482.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747505&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=482

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

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

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

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume