Cyclohexene, 1-ethyl-

Other names:	1-Ethylcyclohexene
	1-Ethylcyclohexene-1
Inchi:	InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h6H,2-5,7H2,1H3
InchiKey:	IFVMAGPISVKRAR-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CCC1=CCCCC1
Mol. weight [g/mol]:	110.20
CAS:	1453-24-3

Physical Properties

Property code	Value	Unit	Source
chl	-5042.18 ± 0.96	kJ/mol	NIST Webbook
gf	68.97	kJ/mol	Joback Method
hf	-63.60	kJ/mol	NIST Webbook
hfl	-106.80 ± 1.00	kJ/mol	NIST Webbook
hfus	8.07	kJ/mol	Joback Method
hvap	43.22	kJ/mol	NIST Webbook
ie	8.48 ± 0.01	eV	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	864.10		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	859.40		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	861.00		NIST Webbook

rinpol	866.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	864.00		NIST Webbook
ripol	1005.30		NIST Webbook
ripol	1013.90		NIST Webbook
ripol	1022.70		NIST Webbook
ripol	1013.90		NIST Webbook
ripol	1022.70		NIST Webbook
ripol	1014.00		NIST Webbook
ripol	1005.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1005.30		NIST Webbook
ripol	1023.00		NIST Webbook
tb	409.90 ± 2.00	K	NIST Webbook
tb	410.20	K	NIST Webbook
tb	408.00 ± 5.00	K	NIST Webbook
tb	408.00 ± 5.00	K	NIST Webbook
tb	408.40 ± 2.00	K	NIST Webbook
tb	408.00 ± 4.00	K	NIST Webbook
tb	409.00 ± 4.00	K	NIST Webbook
tb	409.40 ± 0.60	K	NIST Webbook
tb	409.30 ± 2.00	K	NIST Webbook
tc	615.86	K	Joback Method
tf	163.15 ± 0.06	K	NIST Webbook
tf	163.19 ± 0.02	K	NIST Webbook
tf	163.16 ± 0.04	K	NIST Webbook
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.24	J/mol×K	581.68	Joback Method
cpg	258.76	J/mol×K	547.51	Joback Method
cpg	245.58	J/mol×K	513.33	Joback Method
cpg	231.66	J/mol×K	479.15	Joback Method
cpg	217.00	J/mol×K	444.98	Joback Method
cpg	201.55	J/mol×K	410.80	Joback Method
cpg	283.04	J/mol×K	615.86	Joback Method
dvisc	0.0060480	Pa×s	204.82	Joback Method
dvisc	0.0002579	Pa×s	410.80	Joback Method
dvisc	0.0003434	Pa×s	376.47	Joback Method

dvisc	0.0004841	Pa×s	342.14	Joback Method
dvisc	0.0007368	Pa×s	307.81	Joback Method
dvisc	0.0012462	Pa×s	273.48	Joback Method
dvisc	0.0024511	Pa×s	239.15	Joback Method
hvapt	39.10	kJ/mol	382.50	NIST Webbook
hvapt	40.10	kJ/mol	371.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40053e+01
Coeff. B	-3.24405e+03
Coeff. C	-6.34100e+01
Temperature range (K), min.	299.90
Temperature range (K), max.	436.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00543e+02
Coeff. B	-8.51149e+03
Coeff. C	-1.27413e+01
Coeff. D	8.83219e-06
Temperature range (K), min.	332.15
Temperature range (K), max.	410.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1453243&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=636

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/mol636.mol

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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume