Cyclohexane, 1-ethyl-1-methyl-

Other names:	1-EHTYL-1-METHYLCYCLOHEXANE
	1-Ethyl-1-methylcyclohexane
	1-Methyl-1-ethylcyclohexane
Inchi:	InChI=1S/C9H18/c1-3-9(2)7-5-4-6-8-9/h3-8H2,1-2H3
InchiKey:	YPJRYQGOKHKNKZ-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCC1(C)CCCCC1
Mol. weight [g/mol]:	126.24
CAS:	4926-90-3

Physical Properties

Property code	Value	Unit	Source
chl	-5873.88 ± 0.92	kJ/mol	NIST Webbook
gf	43.86	kJ/mol	Joback Method
hf	-159.53	kJ/mol	Joback Method
hfl	-240.20 ± 1.00	kJ/mol	NIST Webbook
hfus	4.60	kJ/mol	Joback Method
hvap	34.91	kJ/mol	Joback Method
ie	9.34	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	908.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	907.10		NIST Webbook
rinpol	901.50		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	897.00		NIST Webbook

rinpol	901.00		NIST Webbook
tb	425.11	K	Joback Method
tc	633.08	K	Joback Method
tf	222.47	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.14	J/mol×K	425.11	Joback Method
cpg	275.37	J/mol×K	459.77	Joback Method
cpg	293.34	J/mol×K	494.43	Joback Method
cpg	310.16	J/mol×K	529.10	Joback Method
cpg	325.92	J/mol×K	563.76	Joback Method
cpg	340.73	J/mol×K	598.42	Joback Method
cpg	354.69	J/mol×K	633.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42194e+01
Coeff. B	-3.66859e+03
Coeff. C	-4.30990e+01
Temperature range (K), min.	306.42
Temperature range (K), max.	454.93

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol561.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4926903&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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