cis-1-Ethyl-3-methyl-cyclohexane

Other names:	1-Ethyl-3-methylcyclohexane, (Z)-
	1-Ethyl-3-methylcyclohexane, cis
	1-METHYL-CIS-3-ETHYLCYCLOHEXANE
	1-Methyl,cis-3-ethylcyclohexane
	CIS-1-METHYL-3-ETHYLCYCLOHEXANE
	Cyclohexane, 1-ethyl-3-methyl-, cis-
	c-1-Ethyl-3-methylcyclohexane
Inchi:	InChI=1S/C9H18/c1-3-9-6-4-5-8(2)7-9/h8-9H,3-7H2,1-2H3/t8-,9+/m0/s1
InchiKey:	UDDVMPHNQKRNNS-DTWKUNHWSA-N
Formula:	C9H18
SMILES:	CCC1CCCC(C)C1
Mol. weight [g/mol]:	126.24
CAS:	19489-10-2

Physical Properties

Property code	Value	Unit	Source
chl	-5867.30 ± 1.10	kJ/mol	NIST Webbook
gf	41.64	kJ/mol	Joback Method
hf	-195.11	kJ/mol	Joback Method
hfl	-246.70 ± 1.30	kJ/mol	NIST Webbook
hfus	11.97	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	893.70		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	882.78		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	887.00		NIST Webbook

rinpol	914.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	893.70		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	885.20		NIST Webbook
rinpol	889.90		NIST Webbook
rinpol	889.90		NIST Webbook
tb	418.65 ± 2.00	K	NIST Webbook
tb	420.65 ± 1.00	K	NIST Webbook
tb	423.00 ± 2.00	K	NIST Webbook
tb	421.65 ± 2.00	K	NIST Webbook
tb	423.00 ± 3.00	K	NIST Webbook
tb	420.70 ± 2.00	K	NIST Webbook
tb	420.65 ± 1.00	K	NIST Webbook
tb	429.20	K	NIST Webbook
tb	422.40 ± 1.00	K	NIST Webbook
tc	618.70	K	Joback Method
tf	194.33	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.76	J/mol×K	618.70	Joback Method
cpg	340.98	J/mol×K	585.62	Joback Method
cpg	325.42	J/mol×K	552.53	Joback Method
cpg	309.07	J/mol×K	519.45	Joback Method
cpg	291.90	J/mol×K	486.37	Joback Method
cpg	273.91	J/mol×K	453.28	Joback Method
cpg	255.07	J/mol×K	420.20	Joback Method
dvisc	0.0046654	Pa×s	194.33	Joback Method
dvisc	0.0002668	Pa×s	420.20	Joback Method
dvisc	0.0003400	Pa×s	382.56	Joback Method
dvisc	0.0004567	Pa×s	344.91	Joback Method
dvisc	0.0006594	Pa×s	307.26	Joback Method

dvisc	0.0010552	Pa×s	269.62	Joback Method
dvisc	0.0019666	Pa×s	231.97	Joback Method
hvapt	39.00	kJ/mol	419.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.98029e+01
Coeff. B	-7.76031e+03
Coeff. C	-9.55485e+00
Coeff. D	5.46792e-06
Temperature range (K), min.	348.15
Temperature range (K), max.	464.15

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=564
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19489102&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=564
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
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
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