

Cyclohexane, 1-ethyl-2-methyl-, cis-

Other names:	1-Methyl-cis-2-ethylcyclohexane c-1-Ethyl-2-methylcyclohexane cis-1-Ethyl-2-methyl-cyclohexane cis-2-Methyl-1-ethylcyclohexane
Inchi:	InChI=1S/C9H18/c1-3-9-7-5-4-6-8(9)2/h8-9H,3-7H2,1-2H3/t8-,9+/m1/s1
InchiKey:	XARGIVYWQPXRTC-BDAKNGLRSA-N
Formula:	C9H18
SMILES:	CCC1CCCCC1C
Mol. weight [g/mol]:	126.24
CAS:	4923-77-7

Physical Properties

Property code	Value	Unit	Source
chl	-5877.85 ± 0.92	kJ/mol	NIST Webbook
gf	41.64	kJ/mol	Joback Method
hf	-195.11	kJ/mol	Joback Method
hfl	-236.20 ± 1.10	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	923.00		NIST Webbook
rinpol	924.80		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	915.20		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	928.00		NIST Webbook
tb	426.15 ± 2.00	K	NIST Webbook

tb	428.15 ± 2.00	K	NIST Webbook
tb	429.12 ± 0.50	K	NIST Webbook
tb	429.13 ± 0.25	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	255.07	J/mol×K	420.20	Joback Method
cpg	273.91	J/mol×K	453.28	Joback Method
cpg	291.90	J/mol×K	486.37	Joback Method
cpg	309.07	J/mol×K	519.45	Joback Method
cpg	325.42	J/mol×K	552.53	Joback Method
cpg	340.98	J/mol×K	585.62	Joback Method
cpg	355.76	J/mol×K	618.70	Joback Method
dvisc	0.0046654	Pa×s	194.33	Joback Method
dvisc	0.0019666	Pa×s	231.97	Joback Method
dvisc	0.0010552	Pa×s	269.62	Joback Method
dvisc	0.0006594	Pa×s	307.26	Joback Method
dvisc	0.0004567	Pa×s	344.91	Joback Method
dvisc	0.0003400	Pa×s	382.56	Joback Method
dvisc	0.0002668	Pa×s	420.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37991e+01
Coeff. B	-3.31456e+03
Coeff. C	-6.80990e+01
Temperature range (K), min.	313.41
Temperature range (K), max.	458.61

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4923777&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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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