Cyclohexene, 4-ethenyl-

Other names:	1,2,3,4-Tetrahydrostyrene
	1-Cyclohexene, 4-vinyl-
	1-Vinyl-3-cyclohexene
	1-Vinylcyclohex-3-ene
	1-Vinylcyclohexene-3
	4-ETHENYLCYCLOHEXENE
	4-Ethenyl-1-cyclohexene
	4-VINYL-1-CYCLOHEXENE
	4-VINYLCYCLOHEXENE
	4-Vinylcyclohexene-1
	Butadiene dimer
	Cyclohexene, 4-vinyl-
	Cyclohexenylethylene
	NCI-C54999
	NSC 15760
	Vinylcyclohexene
Inchi:	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h2-4,8H,1,5-7H2
InchiKey:	BBDKZWKEPDTENS-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C=CC1CC=CCC1
Mol. weight [g/mol]:	108.18
CAS:	100-40-3

Physical Properties

Property code	Value	Unit	Source
chl	-4889.80	kJ/mol	NIST Webbook
chl	-4892.90 ± 1.30	kJ/mol	NIST Webbook
gf	158.73	kJ/mol	Joback Method
hf	69.50 ± 1.50	kJ/mol	NIST Webbook
hfl	29.70 ± 1.30	kJ/mol	NIST Webbook
hfus	8.25	kJ/mol	Joback Method
hvap	39.80	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
hvap	39.61	kJ/mol	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
ie	8.93 ± 0.02	eV	NIST Webbook
log10ws	-2.53		Crippen Method

logp	2.529		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	120.10		NIST Webbook
rinpol	850.30		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	829.50		NIST Webbook
rinpol	825.10		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	838.10		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	824.00		NIST Webbook
ripol	1039.00		NIST Webbook
tb	402.20	K	NIST Webbook
tb	399.70	K	NIST Webbook
tb	403.20 ± 2.00	K	NIST Webbook
tc	605.48	K	Joback Method
tf	186.30	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.16	J/mol×K	501.66	Joback Method
cpg	266.50	J/mol×K	605.48	Joback Method
cpg	254.79	J/mol×K	570.87	Joback Method
cpg	242.36	J/mol×K	536.27	Joback Method
cpg	184.71	J/mol×K	397.83	Joback Method
cpg	200.36	J/mol×K	432.44	Joback Method
cpg	215.17	J/mol×K	467.05	Joback Method
dvisc	0.0002575	Pa×s	397.83	Joback Method
dvisc	0.0006558	Pa×s	292.07	Joback Method
dvisc	0.0004491	Pa×s	327.32	Joback Method
dvisc	0.0003310	Pa×s	362.58	Joback Method
dvisc	0.0048287	Pa×s	186.30	Joback Method
dvisc	0.0020084	Pa×s	221.56	Joback Method
dvisc	0.0010628	Pa×s	256.81	Joback Method
hvapt	40.10	kJ/mol	348.50	NIST Webbook
hvapt	33.50	kJ/mol	402.20	NIST Webbook
pvap	100.00	kPa	401.42	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z,E-2-Methyl-2-butenenitrile, R,S-4-Vinyl-1-cyclohexene, and Z,E-3-Pentenenitrile
pvap	50.00	kPa	377.75	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z,E-2-Methyl-2-butenenitrile, R,S-4-Vinyl-1-cyclohexene, and Z,E-3-Pentenenitrile

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36542e+01
Coeff. B	-3.31338e+03

Coeff. C	-4.43130e+01
Temperature range (K), min.	292.20
Temperature range (K), max.	441.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.18966e+02
Coeff. B	-8.81256e+03
Coeff. C	-1.57779e+01
Coeff. D	1.35197e-05
Temperature range (K), min.	164.00
Temperature range (K), max.	599.00

Sources

Relation between characteristic molecular volume and hydrophobicity of nonpolar molecules:	https://www.doi.org/10.1016/j.jct.2010.04.011
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=633
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric Vapor Liquid Equilibria for Binary Mixtures of Z|E-2-Methyl-2-butenenitrile, RS-4-Vinyl-1-cyclohexene, and Z-E-3-Pentenenitrile:	https://www.doi.org/10.1021/acs.jced.6b00388
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamics of solvation in propylene glycol and methyl cellosolve:	https://www.doi.org/10.1016/j.jct.2014.06.006
Vapor-Liquid Equilibrium for Binary Mixtures of 3-Cyano-1-butene + RS-4-Vinyl-1-cyclohexene, 3-Cyano-1-butene + ZE-1-Cyano-2-butene and RS-4-Vinyl-1-cyclohexene + ZE-1-Cyano-2-butene:	https://www.doi.org/10.1021/acs.jced.8b00158
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=633
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100403&Units=SI
Vapour pressures and isobaric (vapour + liquid) equilibrium data for the binary system of (RS-4-vinyl-1-cyclohexene + ZE-3-pentenenitrile) at (50.0 and 100.0) kPa:	https://www.doi.org/10.1016/j.jct.2015.08.015

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