

# 4-Ethylcyclohexene

<b>Other names:</b>	1-Ethyl-3-cyclohexene 4-Ethylcyclohexene-1 Cyclohexene, 4-ethyl-
<b>Inchi:</b>	InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h3-4,8H,2,5-7H2,1H3
<b>InchiKey:</b>	CFOHRCNONSEVOJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H14
<b>SMILES:</b>	CCC1CC=CCC1
<b>Mol. weight [g/mol]:</b>	110.20
<b>CAS:</b>	3742-42-5

## Physical Properties

Property code	Value	Unit	Source
gf	70.89	kJ/mol	Joback Method
hf	-96.35	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	34.12	kJ/mol	Joback Method
ie	8.88 ± 0.01	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.753		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	886.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	845.30		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	825.50		NIST Webbook
rinpol	825.50		NIST Webbook
rinpol	851.30		NIST Webbook
rinpol	845.00		NIST Webbook

ripol	988.00		NIST Webbook
ripol	998.90		NIST Webbook
ripol	1009.20		NIST Webbook
ripol	988.00		NIST Webbook
ripol	998.90		NIST Webbook
ripol	1009.20		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	988.00		NIST Webbook
ripol	1009.00		NIST Webbook
tb	401.15	K	Joback Method
tc	604.14	K	Joback Method
tf	188.06	K	Joback Method
vc	0.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.84	J/molxK	401.15	Joback Method
cpg	216.08	J/molxK	434.98	Joback Method
cpg	231.52	J/molxK	468.81	Joback Method
cpg	246.17	J/molxK	502.64	Joback Method
cpg	260.07	J/molxK	536.48	Joback Method
cpg	273.23	J/molxK	570.31	Joback Method
cpg	285.67	J/molxK	604.14	Joback Method
dvisc	0.0057600	Paxs	188.06	Joback Method
dvisc	0.0022895	Paxs	223.57	Joback Method
dvisc	0.0011720	Paxs	259.09	Joback Method
dvisc	0.0007050	Paxs	294.61	Joback Method
dvisc	0.0004731	Paxs	330.12	Joback Method
dvisc	0.0003431	Paxs	365.63	Joback Method
dvisc	0.0002634	Paxs	401.15	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.45486e+01
Coeff. B	-3.37911e+03
Coeff. C	-5.94200e+01
Temperature range (K), min.	296.37
Temperature range (K), max.	425.24

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=638">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=638</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3742425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3742425&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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