

Cyclohexane, ethylidene-

Other names:	Ethylidenecyclohexane
Inchi:	InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h2H,3-7H2,1H3
InchiKey:	BPBOWYWUOUJKLO-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC=C1CCCCC1
Mol. weight [g/mol]:	110.20
CAS:	1003-64-1

Physical Properties

Property code	Value	Unit	Source
chl	-5045.40 ± 0.59	kJ/mol	NIST Webbook
gf	94.10	kJ/mol	Joback Method
hf	-57.76	kJ/mol	Joback Method
hfl	-103.60 ± 0.75	kJ/mol	NIST Webbook
hfus	7.56	kJ/mol	Joback Method
hvap	42.00 ± 0.20	kJ/mol	NIST Webbook
hvap	42.00 ± 0.30	kJ/mol	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.47 ± 0.02	eV	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcpol	108.420	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	873.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	865.90		NIST Webbook
rinpol	861.80		NIST Webbook
rinpol	899.70		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	869.00		NIST Webbook

rinpol	884.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
tb	413.30	K	Joback Method
tc	622.66	K	Joback Method
tf	201.90	K	Joback Method
vc	0.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.71	J/mol×K	413.30	Joback Method
cpg	216.71	J/mol×K	448.19	Joback Method
cpg	231.85	J/mol×K	483.09	Joback Method
cpg	246.17	J/mol×K	517.98	Joback Method
cpg	259.69	J/mol×K	552.87	Joback Method
cpg	272.46	J/mol×K	587.76	Joback Method
cpg	284.49	J/mol×K	622.66	Joback Method
cpl	203.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0068897	Paxs	201.90	Joback Method
dvisc	0.0025992	Paxs	237.13	Joback Method
dvisc	0.0012618	Paxs	272.37	Joback Method
dvisc	0.0007229	Paxs	307.60	Joback Method
dvisc	0.0004644	Paxs	342.83	Joback Method
dvisc	0.0003239	Paxs	378.07	Joback Method
dvisc	0.0002403	Paxs	413.30	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003641&Units=SI>

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
cpl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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