

Cyclohexene, 3-ethenyl-

Inchi:	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h2,4,6,8H,1,3,5,7H2
InchiKey:	YYTUUFMWKBIPEY-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C=CC1C=CCCC1
Mol. weight [g/mol]:	108.18
CAS:	766-03-0

Physical Properties

Property code	Value	Unit	Source
gf	158.73	kJ/mol	Joback Method
hf	29.08	kJ/mol	Joback Method
hfus	8.25	kJ/mol	Joback Method
hvap	33.45	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.529		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	833.00		NIST Webbook
tb	401.90 ± 0.40	K	NIST Webbook
tb	401.90 ± 0.80	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	184.71	J/mol×K	397.83	Joback Method
cpg	254.79	J/mol×K	570.87	Joback Method
cpg	242.36	J/mol×K	536.27	Joback Method
cpg	229.16	J/mol×K	501.66	Joback Method
cpg	215.17	J/mol×K	467.05	Joback Method

cpg	200.36	J/mol×K	432.44	Joback Method
cpg	266.50	J/mol×K	605.48	Joback Method
dvisc	0.0002575	Pa×s	397.83	Joback Method
dvisc	0.0003310	Pa×s	362.58	Joback Method
dvisc	0.0004491	Pa×s	327.32	Joback Method
dvisc	0.0006558	Pa×s	292.07	Joback Method
dvisc	0.0010628	Pa×s	256.81	Joback Method
dvisc	0.0020084	Pa×s	221.56	Joback Method
dvisc	0.0048287	Pa×s	186.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C766030&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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