

# Cyclohexene, 4-ethynyl

<b>Inchi:</b>	InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h1,3-4,8H,5-7H2
<b>InchiKey:</b>	ATMSQOAHGUFOMY-UHFFFAOYSA-N
<b>Formula:</b>	C8H10
<b>SMILES:</b>	C#CC1CC=CCC1
<b>Mol. weight [g/mol]:</b>	106.17

## Physical Properties

Property code	Value	Unit	Source
gf	293.96	kJ/mol	Joback Method
hf	195.55	kJ/mol	Joback Method
hfus	12.51	kJ/mol	Joback Method
hvap	33.98	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.976		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	822.00		NIST Webbook
tb	391.27	K	Joback Method
tc	610.33	K	Joback Method
tf	235.03	K	Joback Method
vc	0.364	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.69	J/mol×K	391.27	Joback Method
cpg	188.48	J/mol×K	427.78	Joback Method
cpg	202.39	J/mol×K	464.29	Joback Method
cpg	215.47	J/mol×K	500.80	Joback Method
cpg	227.74	J/mol×K	537.31	Joback Method
cpg	239.25	J/mol×K	573.82	Joback Method
cpg	250.02	J/mol×K	610.33	Joback Method

# 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>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=R128164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R128164&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>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>rinpol:</b>	Non-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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