

# Cyclohexanol, 1-ethynyl-

<b>Other names:</b>	(1-Hydroxycyclohexyl)ethyne 1-Ethynyl-1-cyclohexanol 1-Ethynyl-1-hydroxycyclohexane 1-Ethynylcyclohexan-1-ol 1-Ethynylcyclohexanol Ethynylcyclohexanol 1-Hydroxy-1-ethynylcyclohexane
<b>Inchi:</b>	InChI=1S/C8H12O/c1-2-8(9)6-4-3-5-7-8/h1,9H,3-7H2
<b>InchiKey:</b>	QYLFHLNFIHBCPR-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O
<b>SMILES:</b>	C#CC1(O)CCCCC1
<b>Mol. weight [g/mol]:</b>	124.18
<b>CAS:</b>	78-27-3

## Physical Properties

Property code	Value	Unit	Source
gf	121.69	kJ/mol	Joback Method
hf	0.78	kJ/mol	Joback Method
hfus	9.08	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
ie	10.60	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	1.315		Crippen Method
mvol	109.990	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	453.20	K	NIST Webbook
tc	697.51	K	Joback Method
tf	305.00 ± 3.00	K	NIST Webbook
vc	0.396	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.68	J/mol×K	484.53	Joback Method

cpg	255.15	J/mol×K	520.03	Joback Method
cpg	267.63	J/mol×K	555.52	Joback Method
cpg	279.22	J/mol×K	591.02	Joback Method
cpg	290.04	J/mol×K	626.52	Joback Method
cpg	300.19	J/mol×K	662.01	Joback Method
cpg	309.80	J/mol×K	697.51	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.00	K	1.60	NIST Webbook

## Sources

<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=C78273&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C78273&amp;Units=SI</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>
<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>

## 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>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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