

# 1-Ethynyl-1-cyclooctanol

<b>Other names:</b>	Cyclooctanol, 1-ethynyl- 1-Aethynyl-cyclooctanol-(1) 1-Ethynylcyclooctanol
<b>Inchi:</b>	InChI=1S/C10H16O/c1-2-10(11)8-6-4-3-5-7-9-10/h1,11H,3-9H2
<b>InchiKey:</b>	DHAPUKCAOFQTIT-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	C#CC1(O)CCCCCCC1
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	55373-76-7

## Physical Properties

Property code	Value	Unit	Source
gf	114.33	kJ/mol	Joback Method
hf	-52.82	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.095		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	538.83	K	Joback Method
tc	760.81	K	Joback Method
tf	334.49	K	Joback Method
vc	0.491	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.58	J/mol×K	538.83	Joback Method
cpg	348.47	J/mol×K	575.83	Joback Method
cpg	364.26	J/mol×K	612.82	Joback Method
cpg	379.07	J/mol×K	649.82	Joback Method
cpg	392.99	J/mol×K	686.81	Joback Method
cpg	406.16	J/mol×K	723.81	Joback Method

cpg

418.69

J/mol×K

760.81

Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.00 ± 1.00	K	1.60	NIST Webbook

## Sources

<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>
<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=C55373767&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373767&amp;Units=SI</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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