

# 4-Hydroxy-non-2-ynoic acid, ethyl ester

<b>Inchi:</b>	InChI=1S/C11H18O3/c1-3-5-6-7-10(12)8-9-11(13)14-4-2/h10,12H,3-7H2,1-2H3
<b>InchiKey:</b>	UHIJSVJMDAUUNM-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O3
<b>SMILES:</b>	CCCCC(O)C#CC(=O)OCC
<b>Mol. weight [g/mol]:</b>	198.26

## Physical Properties

Property code	Value	Unit	Source
gf	-128.64	kJ/mol	Joback Method
hf	-400.38	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	67.68	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.494		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	628.11	K	Joback Method
tc	813.09	K	Joback Method
tf	437.81	K	Joback Method
vc	0.650	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.90	J/molxK	628.11	Joback Method
cpg	450.40	J/molxK	658.94	Joback Method
cpg	462.32	J/molxK	689.77	Joback Method
cpg	473.69	J/molxK	720.60	Joback Method
cpg	484.50	J/molxK	751.43	Joback Method
cpg	494.77	J/molxK	782.26	Joback Method
cpg	504.50	J/molxK	813.09	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=U192422&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U192422&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>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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