

# Hex-4-yn-3-one

<b>Other names:</b>	4-Hexyne-3-one 4-Hexyn-3-one
<b>Inchi:</b>	InChI=1S/C6H8O/c1-3-5-6(7)4-2/h4H2,1-2H3
<b>InchiKey:</b>	BIWUZTZFFUMZIG-UHFFFAOYSA-N
<b>Formula:</b>	C6H8O
<b>SMILES:</b>	CC#CC(=O)CC
<b>Mol. weight [g/mol]:</b>	96.13
<b>CAS:</b>	10575-41-4

## Physical Properties

Property code	Value	Unit	Source
gf	73.52	kJ/mol	Joback Method
hf	-7.45	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	37.85	kJ/mol	Joback Method
ie	9.62	eV	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.989		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	399.55	K	Joback Method
tc	603.51	K	Joback Method
tf	313.41	K	Joback Method
vc	0.340	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.90	J/molxK	399.55	Joback Method
cpg	160.46	J/molxK	433.54	Joback Method
cpg	168.68	J/molxK	467.54	Joback Method
cpg	176.55	J/molxK	501.53	Joback Method
cpg	184.07	J/molxK	535.52	Joback Method
cpg	191.27	J/molxK	569.52	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10575414&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10575414&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>
<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>

## 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>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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