

# 4,6-Heptadiyn-3-one

Inchi:	InChI=1S/C7H6O/c1-3-5-6-7(8)4-2/h1H,4H2,2H3
InchiKey:	TXQOFPBBUQTJSD-UHFFFAOYSA-N
Formula:	C7H6O
SMILES:	C#CC#CC(=O)CC
Mol. weight [g/mol]:	106.12
CAS:	29743-27-9

## Physical Properties

Property code	Value	Unit	Source
gf	305.01	kJ/mol	Joback Method
hf	263.81	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	39.93	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.602		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
tb	412.55	K	Joback Method
tc	630.27	K	Joback Method
tf	371.65	K	Joback Method
vc	0.357	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.09	J/molxK	412.55	Joback Method
cpg	170.16	J/molxK	448.84	Joback Method
cpg	177.80	J/molxK	485.12	Joback Method
cpg	185.03	J/molxK	521.41	Joback Method
cpg	191.88	J/molxK	557.70	Joback Method
cpg	198.35	J/molxK	593.99	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C29743279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29743279&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>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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