

# Hept-3-yn-2-one

<b>Other names:</b>	3-Heptyne-2-one
<b>Inchi:</b>	InChI=1S/C7H10O/c1-3-4-5-6-7(2)8/h3-4H2,1-2H3
<b>InchiKey:</b>	KVCFELYDWWHQI-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O
<b>SMILES:</b>	CCCC#CC(C)=O
<b>Mol. weight [g/mol]:</b>	110.15
<b>CAS:</b>	26059-43-8

## Physical Properties

Property code	Value	Unit	Source
gf	81.94	kJ/mol	Joback Method
hf	-28.09	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	40.07	kJ/mol	Joback Method
ie	9.67	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.379		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	422.43	K	Joback Method
tc	624.38	K	Joback Method
tf	324.68	K	Joback Method
vc	0.396	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.11	J/molxK	422.43	Joback Method
cpg	198.18	J/molxK	456.09	Joback Method
cpg	207.82	J/molxK	489.75	Joback Method
cpg	217.05	J/molxK	523.41	Joback Method
cpg	225.86	J/molxK	557.07	Joback Method
cpg	234.28	J/molxK	590.72	Joback Method
cpg	242.31	J/molxK	624.38	Joback Method

# Sources

<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=C26059438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26059438&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>

# 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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