

# 7-Methyl-6,8-nonadien-2-one

<b>Inchi:</b>	InChI=1S/C10H16O/c1-4-9(2)7-5-6-8-10(3)11/h4,7H,1,5-6,8H2,2-3H3/b9-7+
<b>InchiKey:</b>	KNSKAJBEVXTBQM-VQHVLOKHSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	C=CC(C)=CCCC(C)=O
<b>Mol. weight [g/mol]:</b>	152.23

## Physical Properties

Property code	Value	Unit	Source
gf	63.91	kJ/mol	Joback Method
hf	-129.45	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	43.97	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	1159.00		NIST Webbook
tb	482.79	K	Joback Method
tc	670.35	K	Joback Method
tf	231.59	K	Joback Method
vc	0.564	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.54	J/molxK	482.79	Joback Method
cpg	321.31	J/molxK	514.05	Joback Method
cpg	334.38	J/molxK	545.31	Joback Method
cpg	346.79	J/molxK	576.57	Joback Method
cpg	358.57	J/molxK	607.83	Joback Method
cpg	369.74	J/molxK	639.09	Joback Method
cpg	380.33	J/molxK	670.35	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=R589514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R589514&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>hvac:</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>mccol:</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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