

# (E)-3-Methylnon-2-en-4-one

<b>Inchi:</b>	InChI=1S/C10H18O/c1-4-6-7-8-10(11)9(3)5-2/h5H,4,6-8H2,1-3H3/b9-5+
<b>InchiKey:</b>	OSRWKMOFHSWRRX-WEVVVXLNSA-N
<b>Formula:</b>	C10H18O
<b>SMILES:</b>	CC=C(C)C(=O)CCCCC
<b>Mol. weight [g/mol]:</b>	154.25

## Physical Properties

Property code	Value	Unit	Source
gf	-23.93	kJ/mol	Joback Method
hf	-254.88	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mvol	149.030	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1218.20		NIST Webbook
rinpol	1218.20		NIST Webbook
tb	486.11	K	Joback Method
tc	669.94	K	Joback Method
tf	233.35	K	Joback Method
vc	0.583	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.17	J/molxK	486.11	Joback Method
cpg	339.51	J/molxK	516.75	Joback Method
cpg	353.18	J/molxK	547.39	Joback Method
cpg	366.21	J/molxK	578.03	Joback Method
cpg	378.61	J/molxK	608.66	Joback Method
cpg	390.41	J/molxK	639.30	Joback Method
cpg	401.65	J/molxK	669.94	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=R416243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R416243&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpola:</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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