

# 3,5-Dimethyl-2-octanone

<b>Inchi:</b>	InChI=1S/C10H20O/c1-5-6-8(2)7-9(3)10(4)11/h8-9H,5-7H2,1-4H3
<b>InchiKey:</b>	HSMZFNPREAWEOC-UHFFFAOYSA-N
<b>Formula:</b>	C10H20O
<b>SMILES:</b>	CCCC(C)CC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	156.27
<b>CAS:</b>	19781-14-7

## Physical Properties

Property code	Value	Unit	Source
gf	-100.48	kJ/mol	Joback Method
hf	-372.87	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	43.82	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
tb	481.19	K	Joback Method
tc	661.30	K	Joback Method
tf	222.39	K	Joback Method
vc	0.590	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.29	J/molxK	481.19	Joback Method
cpg	357.47	J/molxK	511.21	Joback Method
cpg	372.01	J/molxK	541.23	Joback Method
cpg	385.92	J/molxK	571.24	Joback Method
cpg	399.22	J/molxK	601.26	Joback Method
cpg	411.92	J/molxK	631.28	Joback Method
cpg	424.04	J/molxK	661.30	Joback Method
dvisc	0.0108635	Paxs	222.39	Joback Method
dvisc	0.0034410	Paxs	265.52	Joback Method

dvisc	0.0015030	Paxs	308.66	Joback Method
dvisc	0.0008043	Paxs	351.79	Joback Method
dvisc	0.0004934	Paxs	394.92	Joback Method
dvisc	0.0003333	Paxs	438.06	Joback Method
dvisc	0.0002415	Paxs	481.19	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781147&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781147&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>dvisc:</b>	Dynamic viscosity
<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>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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