

# 3-Pentanone, 1-phenyl-

<b>Other names:</b>	1-phenylpentan-3-one
<b>Inchi:</b>	InChI=1S/C11H14O/c1-2-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
<b>InchiKey:</b>	GLVAUXMKXKUEEA-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O
<b>SMILES:</b>	CCC(=O)CCc1ccccc1
<b>Mol. weight [g/mol]:</b>	162.23
<b>CAS:</b>	20795-51-1

## Physical Properties

Property code	Value	Unit	Source
gf	25.23	kJ/mol	Joback Method
hf	-146.42	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.598		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	531.63	K	Joback Method
tc	743.09	K	Joback Method
tf	290.08	K	Joback Method
vc	0.549	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.62	J/mol×K	531.63	Joback Method
cpg	387.21	J/mol×K	707.85	Joback Method
cpg	375.71	J/mol×K	672.61	Joback Method
cpg	363.44	J/mol×K	637.36	Joback Method
cpg	350.36	J/mol×K	602.12	Joback Method
cpg	336.43	J/mol×K	566.87	Joback Method

cpg	397.96	J/molxK	743.09	Joback Method
dvisc	0.0002439	Paxs	531.63	Joback Method
dvisc	0.0003133	Paxs	491.37	Joback Method
dvisc	0.0004210	Paxs	451.11	Joback Method
dvisc	0.0005992	Paxs	410.86	Joback Method
dvisc	0.0009211	Paxs	370.60	Joback Method
dvisc	0.0015721	Paxs	330.34	Joback Method
dvisc	0.0031127	Paxs	290.08	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20795511&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20795511&amp;Units=SI</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>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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