

# Methanone, cyclopentylphenyl-

<b>Other names:</b>	Cyclopentyl phenyl ketone Benzoylcyclopentane Ketone, cyclopentyl phenyl Cyclopentanylmethanone
<b>Inchi:</b>	InChI=1S/C12H14O/c13-12(11-8-4-5-9-11)10-6-2-1-3-7-10/h1-3,6-7,11H,4-5,8-9H2
<b>InchiKey:</b>	VYDIMQRLNMMJBW-UHFFFAOYSA-N
<b>Formula:</b>	C12H14O
<b>SMILES:</b>	O=C(c1ccccc1)C1CCCC1
<b>Mol. weight [g/mol]:</b>	174.24
<b>CAS:</b>	5422-88-8

## Physical Properties

Property code	Value	Unit	Source
gf	70.20	kJ/mol	Joback Method
hf	-106.58	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.060		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1508.00		NIST Webbook
tb	569.79	K	Joback Method
tc	810.24	K	Joback Method
tf	312.25	K	Joback Method
vc	0.546	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.87	J/mol×K	569.79	Joback Method
cpg	374.20	J/mol×K	609.86	Joback Method
cpg	391.16	J/mol×K	649.94	Joback Method
cpg	406.83	J/mol×K	690.01	Joback Method

cpg	421.28	J/molxK	730.09	Joback Method
cpg	434.57	J/molxK	770.16	Joback Method
cpg	446.79	J/molxK	810.24	Joback Method
dvisc	0.0033207	Paxs	312.25	Joback Method
dvisc	0.0017664	Paxs	355.17	Joback Method
dvisc	0.0010767	Paxs	398.10	Joback Method
dvisc	0.0007226	Paxs	441.02	Joback Method
dvisc	0.0005206	Paxs	483.94	Joback Method
dvisc	0.0003956	Paxs	526.87	Joback Method
dvisc	0.0003133	Paxs	569.79	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.00 ± 2.00	K	2.10	NIST Webbook

## 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=C5422888&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5422888&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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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