

# 2-Pentanone, 5-(diethylamino)-

<b>Other names:</b>	Novol ketone 5-(Diethylamino)-2-pentanone 5-(N,N-Diethylamino)pentan-2-one DF 493 1-(Diethylamino)-4-pentanone Novalketone 5-Diethylaminopentane-2-one 5-diethylaminopentan-2-one
<b>Inchi:</b>	InChI=1S/C9H19NO/c1-4-10(5-2)8-6-7-9(3)11/h4-8H2,1-3H3
<b>InchiKey:</b>	GRGNJBKJCVOFEO-UHFFFAOYSA-N
<b>Formula:</b>	C9H19NO
<b>SMILES:</b>	CCN(CC)CCCC(C)=O
<b>Mol. weight [g/mol]:</b>	157.25
<b>CAS:</b>	105-14-6

## Physical Properties

Property code	Value	Unit	Source
gf	6.76	kJ/mol	Joback Method
hf	-274.14	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.697		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	471.63	K	Joback Method
tc	644.09	K	Joback Method
tf	273.59	K	Joback Method
vc	0.564	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.21	J/mol×K	471.63	Joback Method

cpg	344.54	J/mol×K	500.37	Joback Method
cpg	358.27	J/mol×K	529.12	Joback Method
cpg	371.39	J/mol×K	557.86	Joback Method
cpg	383.93	J/mol×K	586.60	Joback Method
cpg	395.91	J/mol×K	615.35	Joback Method
cpg	407.34	J/mol×K	644.09	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	2.00	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=C105146&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C105146&amp;Units=SI</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>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

**vc:** Critical Volume

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