

# 2,5-Diethyl cyclopentanone

<b>Inchi:</b>	InChI=1S/C9H16O/c1-3-7-5-6-8(4-2)9(7)10/h7-8H,3-6H2,1-2H3
<b>InchiKey:</b>	CIISROPQPGGRTG-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O
<b>SMILES:</b>	CCC1CCC(CC)C1=O
<b>Mol. weight [g/mol]:</b>	140.22
<b>CAS:</b>	16429-03-1

## Physical Properties

Property code	Value	Unit	Source
gf	-68.85	kJ/mol	Joback Method
hf	-326.65	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	483.75	K	Joback Method
tc	692.38	K	Joback Method
tf	266.07	K	Joback Method
vc	0.486	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.12	J/molxK	483.75	Joback Method
cpg	309.40	J/molxK	518.52	Joback Method
cpg	325.95	J/molxK	553.29	Joback Method
cpg	341.76	J/molxK	588.07	Joback Method
cpg	356.83	J/molxK	622.84	Joback Method
cpg	371.17	J/molxK	657.61	Joback Method
cpg	384.78	J/molxK	692.38	Joback Method

# Sources

<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=C16429031&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16429031&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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