

# 2-Pentenal, 2,4,4-trimethyl-

<b>Other names:</b>	2,4,4-Trimethyl-2-pentenal
<b>Inchi:</b>	InChI=1S/C8H14O/c1-7(6-9)5-8(2,3)4/h5-6H,1-4H3/b7-5+
<b>InchiKey:</b>	ANXYYWCILNEABR-FNORWQNLSA-N
<b>Formula:</b>	C8H14O
<b>SMILES:</b>	CC(C=O)=CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	126.20
<b>CAS:</b>	53907-61-2

## Physical Properties

Property code	Value	Unit	Source
gf	-8.53	kJ/mol	Joback Method
hf	-195.35	kJ/mol	Joback Method
hfus	10.24	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
ripol	1254.00		NIST Webbook
ripol	1254.00		NIST Webbook
tb	431.91	K	Joback Method
tc	626.48	K	Joback Method
tf	205.30	K	Joback Method
vc	0.470	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.32	J/molxK	431.91	Joback Method
cpg	256.71	J/molxK	464.34	Joback Method
cpg	269.30	J/molxK	496.77	Joback Method
cpg	281.13	J/molxK	529.19	Joback Method
cpg	292.25	J/molxK	561.62	Joback Method
cpg	302.69	J/molxK	594.05	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=C53907612&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53907612&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>ripol:</b>	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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