

# 1-Hexene, 2,5,5-trimethyl-

<b>Inchi:</b>	InChI=1S/C9H18/c1-8(2)6-7-9(3,4)5/h1,6-7H2,2-5H3
<b>InchiKey:</b>	GBQMYJAPIDGHKW-UHFFFAOYSA-N
<b>Formula:</b>	C9H18
<b>SMILES:</b>	C=C(C)CCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	126.24
<b>CAS:</b>	62185-56-2

## Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-122.20	kJ/mol	Joback Method
hfus	9.06	kJ/mol	Joback Method
hvap	33.74	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mvol	133.370	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	398.65	K	Joback Method
tc	579.25	K	Joback Method
tf	177.89	K	Joback Method
vc	0.510	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.60	J/mol×K	398.65	Joback Method
cpg	274.01	J/mol×K	428.75	Joback Method
cpg	288.67	J/mol×K	458.85	Joback Method
cpg	302.59	J/mol×K	488.95	Joback Method
cpg	315.80	J/mol×K	519.05	Joback Method
cpg	328.34	J/mol×K	549.15	Joback Method
cpg	340.24	J/mol×K	579.25	Joback Method

# Sources

<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=C62185562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C62185562&amp;Units=SI</a>
<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>

# 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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