

# 2,4,6-Trimethyl-1-nonene, # 2

<b>Other names:</b>	1-Nonene, 2,4,6-trimethyl, # 2
<b>Inchi:</b>	InChI=1S/C12H24/c1-6-7-11(4)9-12(5)8-10(2)3/h11-12H,2,6-9H2,1,3-5H3
<b>InchiKey:</b>	QFMQAIUZMMQKTB-UHFFFAOYSA-N
<b>Formula:</b>	C12H24
<b>SMILES:</b>	C=C(C)CC(C)CC(C)CCC
<b>Mol. weight [g/mol]:</b>	168.32

## Physical Properties

Property code	Value	Unit	Source
gf	124.57	kJ/mol	Joback Method
hf	-185.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.415		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
tb	469.64	K	Joback Method
tc	643.38	K	Joback Method
tf	179.28	K	Joback Method
vc	0.677	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.06	J/molxK	469.64	Joback Method
cpg	406.47	J/molxK	498.60	Joback Method
cpg	423.15	J/molxK	527.55	Joback Method
cpg	439.12	J/molxK	556.51	Joback Method
cpg	454.41	J/molxK	585.47	Joback Method

cpg	469.02	J/mol×K	614.42	Joback Method
cpg	482.99	J/mol×K	643.38	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R529656&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R529656&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>
<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>

## 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>hvp:</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>mvol:</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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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