

# Octane, 2,6,6-trimethyl-

<b>Inchi:</b>	InChI=1S/C11H24/c1-6-11(4,5)9-7-8-10(2)3/h10H,6-9H2,1-5H3
<b>InchiKey:</b>	RUPXAIGHLDMSOL-UHFFFAOYSA-N
<b>Formula:</b>	C11H24
<b>SMILES:</b>	CCC(C)(C)CCCC(C)C
<b>Mol. weight [g/mol]:</b>	156.31
<b>CAS:</b>	54166-32-4

## Physical Properties

Property code	Value	Unit	Source
gf	42.14	kJ/mol	Joback Method
hf	-284.40	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	38.40	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
tb	447.41	K	Joback Method
tc	622.57	K	Joback Method
tf	201.15	K	Joback Method
vc	0.634	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.01	J/molxK	447.41	Joback Method
cpg	443.27	J/molxK	593.38	Joback Method
cpg	428.53	J/molxK	564.18	Joback Method
cpg	413.06	J/molxK	534.99	Joback Method
cpg	396.84	J/molxK	505.80	Joback Method
cpg	379.83	J/molxK	476.60	Joback Method
cpg	457.31	J/molxK	622.57	Joback Method
dvisc	0.0002213	Paxs	447.41	Joback Method
dvisc	0.0003193	Paxs	406.37	Joback Method

dvisc	0.0005003	Paxs	365.32	Joback Method
dvisc	0.0008784	Paxs	324.28	Joback Method
dvisc	0.0018154	Paxs	283.24	Joback Method
dvisc	0.0047986	Paxs	242.19	Joback Method
dvisc	0.0188587	Paxs	201.15	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=C54166324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54166324&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>dvisc:</b>	Dynamic viscosity
<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>mccvol:</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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