

# 3-Hexene, 3-ethyl-2,5-dimethyl-

<b>Inchi:</b>	InChI=1S/C10H20/c1-6-10(9(4)5)7-8(2)3/h7-9H,6H2,1-5H3/b10-7+
<b>InchiKey:</b>	LTFIBGYQLWKTKK-JXMROGBWSA-N
<b>Formula:</b>	C10H20
<b>SMILES:</b>	CCC(=CC(C)C)C(C)C
<b>Mol. weight [g/mol]:</b>	140.27
<b>CAS:</b>	62338-08-3

## Physical Properties

Property code	Value	Unit	Source
gf	100.11	kJ/mol	Joback Method
hf	-152.86	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	37.12	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.635		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
tb	431.36	K	Joback Method
tc	612.63	K	Joback Method
tf	153.42	K	Joback Method
vc	0.565	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.22	J/molxK	431.36	Joback Method
cpg	316.29	J/molxK	461.57	Joback Method
cpg	331.64	J/molxK	491.78	Joback Method
cpg	346.28	J/molxK	522.00	Joback Method
cpg	360.25	J/molxK	552.21	Joback Method
cpg	373.58	J/molxK	582.42	Joback Method
cpg	386.28	J/molxK	612.63	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=C62338083&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C62338083&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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