

# 2,4-Dimethyl-1-hexene

<b>Other names:</b>	1-Hexene, 2,4-dimethyl- 2,4-Dimethyl hexene-1 2,4-Dimethylhex-1-ene <chem>C2H5CH(CH3)CH2C(CH3)=CH2</chem>
<b>Inchi:</b>	InChI=1S/C8H16/c1-5-8(4)6-7(2)3/h8H,2,5-6H2,1,3-4H3
<b>InchiKey:</b>	PKVDGQHNRICJLA-UHFFFAOYSA-N
<b>Formula:</b>	C8H16
<b>SMILES:</b>	<chem>C=C(C)CC(C)CC</chem>
<b>Mol. weight [g/mol]:</b>	112.21
<b>CAS:</b>	16746-87-5

## Physical Properties

Property code	Value	Unit	Source
gf	93.33	kJ/mol	Joback Method
hf	-98.09	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	739.80		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	738.50		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	750.70		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	737.50		NIST Webbook
tb	378.56	K	Joback Method
tc	552.61	K	Joback Method
tf	149.20	K	Joback Method
vc	0.460	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.59	J/molxK	378.56	Joback Method
cpg	230.69	J/molxK	407.57	Joback Method
cpg	243.26	J/molxK	436.58	Joback Method
cpg	255.31	J/molxK	465.59	Joback Method
cpg	266.87	J/molxK	494.59	Joback Method
cpg	277.94	J/molxK	523.60	Joback Method
cpg	288.55	J/molxK	552.61	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32291e+01
Coeff. B	-2.90253e+03
Coeff. C	-5.62750e+01
Temperature range (K), min.	280.55
Temperature range (K), max.	422.86

## Sources

The Yaws Handbook of Vapor Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

KDB:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=284>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C16746875&Units=SI>

# 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>hvac:</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>pvap:</b>	Vapor 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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