

# (E)-3-Methylhept-2-ene

<b>Other names:</b>	(E)-2-Heptene, 3-methyl 2-Heptene, 3-methyl-, (E)- 3-Methyl-trans-2-heptene
<b>Inchi:</b>	InChI=1S/C8H16/c1-4-6-7-8(3)5-2/h5H,4,6-7H2,1-3H3/b8-5+
<b>InchiKey:</b>	OFKLSPUVNMOIJB-VMPITWQZSA-N
<b>Formula:</b>	C8H16
<b>SMILES:</b>	CC=C(C)CCCC
<b>Mol. weight [g/mol]:</b>	112.21
<b>CAS:</b>	22768-20-3

## Physical Properties

Property code	Value	Unit	Source
gf	88.15	kJ/mol	Joback Method
hf	-101.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	39.70	kJ/mol	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	797.00		NIST Webbook
rinpol	797.50		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	797.20		NIST Webbook
rinpol	806.60		NIST Webbook
tb	386.48	K	Joback Method
tc	561.75	K	Joback Method
tf	160.88	K	Joback Method
vc	0.465	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/molxK	386.48	Joback Method
cpg	231.15	J/molxK	415.69	Joback Method
cpg	243.70	J/molxK	444.90	Joback Method
cpg	255.70	J/molxK	474.11	Joback Method
cpg	267.18	J/molxK	503.32	Joback Method
cpg	278.15	J/molxK	532.54	Joback Method
cpg	288.64	J/molxK	561.75	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44013e+01
Coeff. B	-3.37398e+03
Coeff. C	-4.84700e+01
Temperature range (K), min.	287.53
Temperature range (K), max.	419.65

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22768203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22768203&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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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