

# 3-Ethyl-2-methyl-1-heptene

<b>Inchi:</b>	InChI=1S/C10H20/c1-5-7-8-10(6-2)9(3)4/h10H,3,5-8H2,1-2,4H3
<b>InchiKey:</b>	ZNQRZLWSGCOUEI-UHFFFAOYSA-N
<b>Formula:</b>	C10H20
<b>SMILES:</b>	C=C(C)C(CC)CCCC
<b>Mol. weight [g/mol]:</b>	140.27
<b>CAS:</b>	19780-60-0

## Physical Properties

Property code	Value	Unit	Source
gf	110.17	kJ/mol	Joback Method
hf	-139.37	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	36.88	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1098.40		NIST Webbook
tb	424.32	K	Joback Method
tc	596.75	K	Joback Method
tf	171.74	K	Joback Method
vc	0.572	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.04	J/mol×K	424.32	Joback Method
cpg	314.31	J/mol×K	453.06	Joback Method
cpg	328.96	J/mol×K	481.80	Joback Method
cpg	343.01	J/mol×K	510.54	Joback Method
cpg	356.47	J/mol×K	539.27	Joback Method
cpg	369.36	J/mol×K	568.01	Joback Method
cpg	381.70	J/mol×K	596.75	Joback Method

# 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C19780600&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780600&amp;Units=SI</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</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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