

# 3-Heptyne, 5-ethyl-5-methyl-

<b>Other names:</b>	5-ethyl-5-methyl-3-heptyne
<b>Inchi:</b>	InChI=1S/C10H18/c1-5-8-9-10(4,6-2)7-3/h5-7H2,1-4H3
<b>InchiKey:</b>	YHNZUFTUGJAEPN-UHFFFAOYSA-N
<b>Formula:</b>	C10H18
<b>SMILES:</b>	CCC#CC(C)(CC)CC
<b>Mol. weight [g/mol]:</b>	138.25
<b>CAS:</b>	61228-10-2

## Physical Properties

Property code	Value	Unit	Source
gf	238.96	kJ/mol	Joback Method
hf	13.82	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	38.71	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.226		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	433.97	K	Joback Method
tc	630.64	K	Joback Method
tf	310.98	K	Joback Method
vc	0.546	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.42	J/mol×K	433.97	Joback Method
cpg	306.36	J/mol×K	466.75	Joback Method
cpg	321.48	J/mol×K	499.53	Joback Method
cpg	335.83	J/mol×K	532.31	Joback Method
cpg	349.43	J/mol×K	565.08	Joback Method
cpg	362.32	J/mol×K	597.86	Joback Method
cpg	374.53	J/mol×K	630.64	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50814e+01
Coeff. B	-4.00075e+03
Coeff. C	-6.44840e+01
Temperature range (K), min.	334.92
Temperature range (K), max.	473.98

## 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=C61228102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61228102&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>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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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