

# Hexanoic acid, 2-methyloct-5-yn-4-yl ester

<b>Inchi:</b>	InChI=1S/C15H26O2/c1-5-7-9-11-15(16)17-14(10-8-6-2)12-13(3)4/h13-14H,5-7,9,11-12H
<b>InchiKey:</b>	MUXKWTODTLREAC-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O2
<b>SMILES:</b>	CCC#CC(CC(C)C)OC(=O)CCCCC
<b>Mol. weight [g/mol]:</b>	238.37

## Physical Properties

Property code	Value	Unit	Source
gf	39.42	kJ/mol	Joback Method
hf	-335.99	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.938		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpola	1526.00		NIST Webbook
rinpola	1526.00		NIST Webbook
tb	627.01	K	Joback Method
tc	816.50	K	Joback Method
tf	407.07	K	Joback Method
vc	0.850	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.84	J/molxK	627.01	Joback Method
cpg	599.50	J/molxK	658.59	Joback Method
cpg	616.33	J/molxK	690.17	Joback Method
cpg	632.35	J/molxK	721.76	Joback Method
cpg	647.57	J/molxK	753.34	Joback Method
cpg	662.00	J/molxK	784.92	Joback Method
cpg	675.67	J/molxK	816.50	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=U299356&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299356&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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