

# 1-Phenyl-1-nonyne

<b>Inchi:</b>	InChI=1S/C15H20/c1-2-3-4-5-6-7-9-12-15-13-10-8-11-14-15/h8,10-11,13-14H,2-7H2,1H3
<b>InchiKey:</b>	ZRQWNFWWPPYNFA-UHFFFAOYSA-N
<b>Formula:</b>	C15H20
<b>SMILES:</b>	CCCCCCCC#Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	200.32
<b>CAS:</b>	57718-18-0

## Physical Properties

Property code	Value	Unit	Source
gf	390.63	kJ/mol	Joback Method
hf	155.90	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	53.41	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.399		Crippen Method
mcvol	189.850	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
tb	578.28	K	Joback Method
tc	792.85	K	Joback Method
tf	391.33	K	Joback Method
vc	0.730	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.59	J/molxK	578.28	Joback Method
cpg	473.88	J/molxK	614.04	Joback Method
cpg	491.11	J/molxK	649.80	Joback Method
cpg	507.32	J/molxK	685.57	Joback Method
cpg	522.57	J/molxK	721.33	Joback Method
cpg	536.90	J/molxK	757.09	Joback Method
cpg	550.36	J/molxK	792.85	Joback Method

# Sources

<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.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=C57718180&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57718180&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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