

# 2-Pentanol, 5-(2-propynyloxy)-

<b>Other names:</b>	5-(2-propynyloxy)-2-pentanol
<b>Inchi:</b>	InChI=1S/C8H14O2/c1-3-6-10-7-4-5-8(2)9/h1,8-9H,4-7H2,2H3
<b>InchiKey:</b>	GIMRTZTZHZCXQX-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O2
<b>SMILES:</b>	C#CCOCCCC(C)O
<b>Mol. weight [g/mol]:</b>	142.20
<b>CAS:</b>	55702-67-5

## Physical Properties

Property code	Value	Unit	Source
gf	-4.71	kJ/mol	Joback Method
hf	-206.28	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	0.797		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	486.72	K	Joback Method
tc	659.55	K	Joback Method
tf	294.94	K	Joback Method
vc	0.476	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.63	J/molxK	486.72	Joback Method
cpg	291.96	J/molxK	515.53	Joback Method
cpg	301.90	J/molxK	544.33	Joback Method
cpg	311.44	J/molxK	573.14	Joback Method
cpg	320.59	J/molxK	601.94	Joback Method
cpg	329.37	J/molxK	630.75	Joback Method
cpg	337.78	J/molxK	659.55	Joback Method

# Sources

<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=C55702675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55702675&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>

# 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>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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