

# 1,3-Pentadiyne

Inchi:	InChI=1S/C5H4/c1-3-5-4-2/h1H,2H3
InchiKey:	VNMDYSSJFJFEQI-UHFFFAOYSA-N
Formula:	C5H4
SMILES:	C#CC#CC
Mol. weight [g/mol]:	64.09
CAS:	4911-55-1

## Physical Properties

Property code	Value	Unit	Source
gf	417.09	kJ/mol	Joback Method
hf	417.67	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	28.73	kJ/mol	Joback Method
ie	9.51	eV	NIST Webbook
ie	9.50 ± 0.02	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.51	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.643		Crippen Method
mvol	64.110	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	328.00 ± 4.00	K	NIST Webbook
tb	328.70	K	NIST Webbook
tc	516.81	K	Joback Method
tf	299.18	K	Joback Method
vc	0.239	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.77	J/mol×K	312.92	Joback Method
cpg	94.86	J/mol×K	346.90	Joback Method
cpg	99.71	J/mol×K	380.88	Joback Method

cpg	104.32	J/mol×K	414.87	Joback Method
cpg	108.72	J/mol×K	448.85	Joback Method
cpg	112.91	J/mol×K	482.83	Joback Method
cpg	116.90	J/mol×K	516.81	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.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=C4911551&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4911551&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>ie:</b>	Ionization energy
<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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