

# CH3-CC-CC-CH2

**Inchi:** InChI=1S/C6H5/c1-3-5-6-4-2/h1H2,2H3  
**InchiKey:** TZTSOMWOQWNAND-UHFFFAOYSA-N  
**Formula:** C6H5  
**SMILES:** [CH2]C#CC#CC  
**Mol. weight [g/mol]:** 77.10  
**CAS:** 116138-99-9

## Physical Properties

Property code	Value	Unit	Source
affp	819.10	kJ/mol	NIST Webbook
basg	786.60	kJ/mol	NIST Webbook
gf	457.62	kJ/mol	Joback Method
hf	433.24	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	33.11	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.847		Crippen Method
mcvol	76.050	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	353.98	K	Joback Method
tc	569.21	K	Joback Method
tf	385.95	K	Joback Method
vc	0.286	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.51	J/molxK	353.98	Joback Method
cpg	117.25	J/molxK	389.85	Joback Method
cpg	123.52	J/molxK	425.72	Joback Method
cpg	129.38	J/molxK	461.59	Joback Method
cpg	134.84	J/molxK	497.46	Joback Method
cpg	139.96	J/molxK	533.33	Joback Method
cpg	144.76	J/molxK	569.21	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=C116138999&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116138999&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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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