

# 1,4-Diethynylbenzene

<b>Other names:</b>	Benzene,1,4-diethynyl- 1,4-Bis(ethynyl)benzene
<b>Inchi:</b>	InChI=1S/C10H6/c1-3-9-5-7-10(4-2)8-6-9/h1-2,5-8H
<b>InchiKey:</b>	MVLGANVFCMOJHR-UHFFFAOYSA-N
<b>Formula:</b>	C10H6
<b>SMILES:</b>	C#Cc1ccc(C#C)cc1
<b>Mol. weight [g/mol]:</b>	126.15
<b>CAS:</b>	935-14-8

## Physical Properties

Property code	Value	Unit	Source
gf	582.24	kJ/mol	Joback Method
hf	559.13	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	40.51	kJ/mol	Joback Method
ie	8.58 ± 0.02	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	1.649		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	440.10	K	Joback Method
tc	679.89	K	Joback Method
tf	335.34	K	Joback Method
vc	0.411	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.09	J/molxK	440.10	Joback Method
cpg	209.35	J/molxK	480.07	Joback Method
cpg	219.75	J/molxK	520.03	Joback Method
cpg	229.36	J/molxK	560.00	Joback Method
cpg	238.22	J/molxK	599.96	Joback Method
cpg	246.40	J/molxK	639.93	Joback Method

## Sources

<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=C935148&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C935148&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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