

# Benzonitrile, 4-ethenyl-

<b>Other names:</b>	Benzonitrile, p-vinyl- 4-Cyanostyrene 4-Vinylbenzonitrile p-Cyanostyrene p-Vinylbenzonitrile
<b>Inchi:</b>	InChI=1S/C9H7N/c1-2-8-3-5-9(7-10)6-4-8/h2-6H,1H2
<b>InchiKey:</b>	SNTUCKQYWGHPZPK-UHFFFAOYSA-N
<b>Formula:</b>	C9H7N
<b>SMILES:</b>	C=Cc1ccc(C#N)cc1
<b>Mol. weight [g/mol]:</b>	129.16
<b>CAS:</b>	3435-51-6

## Physical Properties

Property code	Value	Unit	Source
gf	348.70	kJ/mol	Joback Method
hf	286.28	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	48.37	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.201		Crippen Method
mcvol	110.990	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	535.74	K	Joback Method
tc	769.53	K	Joback Method
tf	258.15 ± 2.00	K	NIST Webbook
vc	0.439	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.88	J/mol×K	535.74	Joback Method
cpg	235.25	J/mol×K	574.71	Joback Method
cpg	244.91	J/mol×K	613.67	Joback Method
cpg	253.89	J/mol×K	652.64	Joback Method

cpg	262.23	J/mol×K	691.60	Joback Method
cpg	269.96	J/mol×K	730.57	Joback Method
cpg	277.13	J/mol×K	769.53	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=C3435516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3435516&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>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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