

# Benzene, (2-nitroethenyl)-

<b>Other names:</b>	Styrene, «beta»-nitro- «beta»-Nitrostyrene «omega»-Nitrostyrene (2-Nitrovinyl)benzene 1-Nitro-2-phenylethylene 1-Phenyl-2-nitroethene BNS NCI-C02211 2-Nitro-1-phenylethylene Styrene, beta-nitro 2-Nitroethenylbenzene NSC 9809
<b>Inchi:</b>	InChI=1S/C8H7NO2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H
<b>InchiKey:</b>	PIAOLBVUVDXHHL-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO2
<b>SMILES:</b>	O=[N+](O-)C=Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	149.15
<b>CAS:</b>	102-96-5

## Physical Properties

Property code	Value	Unit	Source
chs	-4179.00 ± 2.10	kJ/mol	NIST Webbook
gf	244.66	kJ/mol	Joback Method
hf	134.54	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.934		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	565.12	K	Joback Method
tc	820.37	K	Joback Method
tf	331.00 ± 4.00	K	NIST Webbook
vc	0.438	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.26	J/mol×K	565.12	Joback Method
cpg	258.06	J/mol×K	607.66	Joback Method
cpg	268.84	J/mol×K	650.20	Joback Method
cpg	278.67	J/mol×K	692.75	Joback Method
cpg	287.64	J/mol×K	735.29	Joback Method
cpg	295.84	J/mol×K	777.83	Joback Method
cpg	303.34	J/mol×K	820.37	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=C102965&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C102965&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>chs:</b>	Standard solid enthalpy of combustion
<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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