

# Benzene, 1-bromo-4-ethynyl-

<b>Inchi:</b>	InChI=1S/C8H5Br/c1-2-7-3-5-8(9)6-4-7/h1,3-6H
<b>InchiKey:</b>	LTLVZQZDXQWLHU-UHFFFAOYSA-N
<b>Formula:</b>	C8H5Br
<b>SMILES:</b>	C#Cc1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	181.03
<b>CAS:</b>	766-96-1

## Physical Properties

Property code	Value	Unit	Source
gf	356.65	kJ/mol	Joback Method
hf	334.84	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
ie	8.62	eV	NIST Webbook
log10ws	-3.33		Crippen Method
logp	2.430		Crippen Method
mcvol	108.720	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	470.38	K	Joback Method
tc	718.89	K	Joback Method
tf	325.63	K	Joback Method
vc	0.400	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.23	J/mol×K	470.38	Joback Method
cpg	191.92	J/mol×K	511.80	Joback Method
cpg	200.81	J/mol×K	553.22	Joback Method
cpg	208.97	J/mol×K	594.63	Joback Method
cpg	216.44	J/mol×K	636.05	Joback Method
cpg	223.29	J/mol×K	677.47	Joback Method
cpg	229.58	J/mol×K	718.89	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	2.10	NIST Webbook

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C766961&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C766961&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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