

# Benzene, 1,3-butadienyl-

<b>Other names:</b>	1,3-Butadiene, 1-phenyl- 1-Phenylbutadiene 1-Phenyl-1,3-butadiene 1,3-Butadienylbenzene
<b>Inchi:</b>	InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h2-9H,1H2
<b>InchiKey:</b>	XZKRX PZXQLARHH-UHFFFAOYSA-N
<b>Formula:</b>	C10H10
<b>SMILES:</b>	<chem>C=CC=Cc1ccccc1</chem>
<b>Mol. weight [g/mol]:</b>	130.19
<b>CAS:</b>	1515-78-2

## Physical Properties

Property code	Value	Unit	Source
gf	313.79	kJ/mol	Joback Method
hf	229.45	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	39.42	kJ/mol	Joback Method
ie	8.39	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.886		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	177.00		NIST Webbook
rinpol	1150.00		NIST Webbook
ripol	1572.00		NIST Webbook
tb	455.72	K	Joback Method
tc	675.61	K	Joback Method
tf	222.04	K	Joback Method
vc	0.449	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.50	J/molxK	455.72	Joback Method

cpg	284.74	J/molxK	638.97	Joback Method
cpg	274.22	J/molxK	602.32	Joback Method
cpg	262.90	J/molxK	565.67	Joback Method
cpg	250.71	J/molxK	529.02	Joback Method
cpg	237.60	J/molxK	492.37	Joback Method
cpg	294.51	J/molxK	675.61	Joback Method
dvisc	0.0001896	Paxs	455.72	Joback Method
dvisc	0.0002424	Paxs	416.77	Joback Method
dvisc	0.0003258	Paxs	377.83	Joback Method
dvisc	0.0004689	Paxs	338.88	Joback Method
dvisc	0.0007416	Paxs	299.93	Joback Method
dvisc	0.0013450	Paxs	260.99	Joback Method
dvisc	0.0030060	Paxs	222.04	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=C1515782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1515782&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>dvisc:</b>	Dynamic viscosity
<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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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