

# Benzene, 1,1'-(2-butene-1,4-diyl)bis-

<b>Inchi:</b>	InChI=1S/C16H16/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-12H,13-14H2/b8-7-
<b>InchiKey:</b>	CTYOBVWQEXIGRQ-BQYQJAHWSA-N
<b>Formula:</b>	C16H16
<b>SMILES:</b>	C(=CCc1ccccc1)Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	208.30
<b>CAS:</b>	13657-49-3

## Physical Properties

Property code	Value	Unit	Source
gf	388.88	kJ/mol	Joback Method
hf	216.71	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.028		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1731.60		NIST Webbook
tb	623.00	K	Joback Method
tc	863.17	K	Joback Method
tf	318.40 ± 2.00	K	NIST Webbook
vc	0.696	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.62	J/mol×K	623.00	Joback Method
cpg	469.78	J/mol×K	663.03	Joback Method
cpg	486.53	J/mol×K	703.06	Joback Method
cpg	501.97	J/mol×K	743.09	Joback Method
cpg	516.22	J/mol×K	783.11	Joback Method
cpg	529.37	J/mol×K	823.14	Joback Method
cpg	541.54	J/mol×K	863.17	Joback Method

dvisc	0.0022682	Paxs	317.84	Joback Method
dvisc	0.0010118	Paxs	368.70	Joback Method
dvisc	0.0005489	Paxs	419.56	Joback Method
dvisc	0.0003399	Paxs	470.42	Joback Method
dvisc	0.0002311	Paxs	521.28	Joback Method
dvisc	0.0001683	Paxs	572.14	Joback Method
dvisc	0.0001290	Paxs	623.00	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=C13657493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13657493&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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