

# Benzene, 1,1'-ethenyldienebis-[4-methyl-

<b>Other names:</b>	1,1-di(p-Tolyl)ethylene
<b>Inchi:</b>	InChI=1S/C16H16/c1-12-4-8-15(9-5-12)14(3)16-10-6-13(2)7-11-16/h4-11H,3H2,1-2H3
<b>InchiKey:</b>	HEDMCKGHZIRQLS-UHFFFAOYSA-N
<b>Formula:</b>	C16H16
<b>SMILES:</b>	<chem>C=C(c1ccc(C)cc1)c1ccc(C)cc1</chem>
<b>Mol. weight [g/mol]:</b>	208.30
<b>CAS:</b>	2919-20-2

## Physical Properties

Property code	Value	Unit	Source
affp	900.20	kJ/mol	NIST Webbook
basg	871.40	kJ/mol	NIST Webbook
chs	-8522.00 ± 2.00	kJ/mol	NIST Webbook
chs	-8668.70 ± 2.00	kJ/mol	NIST Webbook
gf	368.69	kJ/mol	Joback Method
hf	192.19	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hsub	101.00 ± 1.40	kJ/mol	NIST Webbook
hvap	56.50	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.365		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
tb	625.36	K	Joback Method
tc	866.59	K	Joback Method
tf	332.24	K	Joback Method
vc	0.698	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.50	J/mol×K	786.18	Joback Method
cpg	526.61	J/mol×K	826.38	Joback Method
cpg	449.64	J/mol×K	625.36	Joback Method

cpg	467.47	J/mol×K	665.56	Joback Method
cpg	484.01	J/mol×K	705.77	Joback Method
cpg	499.32	J/mol×K	745.97	Joback Method
cpg	538.73	J/mol×K	866.59	Joback Method
hfust	23.31	kJ/mol	334.10	NIST Webbook
hsubt	100.30 ± 1.40	kJ/mol	320.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00 ± 1.00	K	0.08	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C2919202&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2919202&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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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>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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