

# Benzene, 1,1'-(1,4-dimethyl-1,4-butanediyl)bis-

<b>Other names:</b>	Hexane, 2,5-diphenyl- 2,5-Diphenylhexane 1,1'-(1,4-dimethyl-1,4-butanediyl)bisbenzene
<b>Inchi:</b>	InChI=1S/C18H22/c1-15(17-9-5-3-6-10-17)13-14-16(2)18-11-7-4-8-12-18/h3-12,15-16H,
<b>InchiKey:</b>	SFGSCWQCLSTTPQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H22
<b>SMILES:</b>	CC(CCC(C)c1ccccc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	238.37
<b>CAS:</b>	3548-85-4

## Physical Properties

Property code	Value	Unit	Source
gf	320.62	kJ/mol	Joback Method
hf	47.65	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	59.44	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.374		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	663.72	K	Joback Method
tc	894.23	K	Joback Method
tf	315.46	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.75	J/mol×K	663.72	Joback Method
cpg	598.84	J/mol×K	702.14	Joback Method
cpg	617.48	J/mol×K	740.56	Joback Method
cpg	634.76	J/mol×K	778.98	Joback Method
cpg	650.76	J/mol×K	817.40	Joback Method
cpg	665.57	J/mol×K	855.81	Joback Method

cpg	679.28	J/mol×K	894.23	Joback Method
dvisc	0.0037813	Paxs	315.46	Joback Method
dvisc	0.0013126	Paxs	373.50	Joback Method
dvisc	0.0006057	Paxs	431.55	Joback Method
dvisc	0.0003357	Paxs	489.59	Joback Method
dvisc	0.0002109	Paxs	547.63	Joback Method
dvisc	0.0001448	Paxs	605.68	Joback Method
dvisc	0.0001062	Paxs	663.72	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3548854&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3548854&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>
<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>

## 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>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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