

# Benzene, 1,1'-(1,6-hexanediyl)bis-

<b>Other names:</b>	Hexane, 1,6-diphenyl- 1,6-Diphenylhexane
<b>Inchi:</b>	InChI=1S/C18H22/c1(5-11-17-13-7-3-8-14-17)2-6-12-18-15-9-4-10-16-18/h3-4,7-10,13-1
<b>InchiKey:</b>	DVGPMIRVCZNXMD-UHFFFAOYSA-N
<b>Formula:</b>	C18H22
<b>SMILES:</b>	<chem>c1ccc(CCCCCC2CCCCC2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	238.37
<b>CAS:</b>	1087-49-6

## Physical Properties

Property code	Value	Unit	Source
affp	826.10	kJ/mol	NIST Webbook
basg	783.80	kJ/mol	NIST Webbook
chl	-10230.00	kJ/mol	NIST Webbook
gf	325.50	kJ/mol	Joback Method
hf	58.21	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.032		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
tb	618.82 ± 0.20	K	NIST Webbook
tc	886.15	K	Joback Method
tf	280.10 ± 2.00	K	NIST Webbook
tf	261.16 ± 0.05	K	NIST Webbook
vc	0.828	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.08	J/mol×K	886.15	Joback Method
cpg	661.65	J/mol×K	849.23	Joback Method
cpg	647.22	J/mol×K	812.30	Joback Method

cpg	631.70	J/molxK	775.38	Joback Method
cpg	615.01	J/molxK	738.45	Joback Method
cpg	597.08	J/molxK	701.53	Joback Method
cpg	577.84	J/molxK	664.60	Joback Method
dvisc	0.0021987	Paxs	345.46	Joback Method
dvisc	0.0001234	Paxs	664.60	Joback Method
dvisc	0.0001618	Paxs	611.41	Joback Method
dvisc	0.0002235	Paxs	558.22	Joback Method
dvisc	0.0003304	Paxs	505.03	Joback Method
dvisc	0.0005356	Paxs	451.84	Joback Method
dvisc	0.0009876	Paxs	398.65	Joback Method
hvapt	88.00	kJ/mol	333.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1087496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1087496&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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

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

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