

# Benzene, 1,1'-(3,3-dimethylbutylidene)bis-

<b>Inchi:</b>	InChI=1S/C18H22/c1-18(2,3)14-17(15-10-6-4-7-11-15)16-12-8-5-9-13-16/h4-13,17H,14H
<b>InchiKey:</b>	LRFSDPAZFHHGLC-UHFFFAOYSA-N
<b>Formula:</b>	C18H22
<b>SMILES:</b>	CC(C)(C)CC(c1ccccc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	238.37
<b>CAS:</b>	57123-34-9

## Physical Properties

Property code	Value	Unit	Source
gf	325.90	kJ/mol	Joback Method
hf	44.18	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	58.53	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.255		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
tb	589.00 ± 8.00	K	NIST Webbook
tb	589.00 ± 6.00	K	NIST Webbook
tc	900.34	K	Joback Method
tf	306.00 ± 4.00	K	NIST Webbook
tf	306.00 ± 4.00	K	NIST Webbook
vc	0.810	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.95	J/mol×K	660.93	Joback Method
cpg	668.97	J/mol×K	860.44	Joback Method
cpg	654.11	J/mol×K	820.53	Joback Method
cpg	638.00	J/mol×K	780.63	Joback Method
cpg	620.52	J/mol×K	740.73	Joback Method
cpg	601.55	J/mol×K	700.83	Joback Method
cpg	682.70	J/mol×K	900.34	Joback Method

dvisc	0.0000981	Paxs	660.93	Joback Method
dvisc	0.0001352	Paxs	606.25	Joback Method
dvisc	0.0001985	Paxs	551.58	Joback Method
dvisc	0.0003172	Paxs	496.90	Joback Method
dvisc	0.0005694	Paxs	442.23	Joback Method
dvisc	0.0012051	Paxs	387.56	Joback Method
dvisc	0.0032634	Paxs	332.88	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57123349&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57123349&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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