

# Benzene, 1,3-bis(1-methylpropyl)-

<b>Other names:</b>	Benzene, m-di-sec-butyl-
<b>Inchi:</b>	InChI=1S/C14H22/c1-5-11(3)13-8-7-9-14(10-13)12(4)6-2/h7-12H,5-6H2,1-4H3
<b>InchiKey:</b>	SGJNVYYELDBNLA-UHFFFAOYSA-N
<b>Formula:</b>	C14H22
<b>SMILES:</b>	CCC(C)c1cccc(C(C)CC)c1
<b>Mol. weight [g/mol]:</b>	190.32
<b>CAS:</b>	1079-96-5

## Physical Properties

Property code	Value	Unit	Source
gf	164.90	kJ/mol	Joback Method
hf	-117.79	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.714		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
ripol	1478.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1477.00		NIST Webbook
tb	550.50	K	Joback Method
tc	753.79	K	Joback Method
tf	256.48	K	Joback Method
vc	0.700	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	442.99	J/molxK	550.50	Joback Method
cpg	527.03	J/molxK	719.91	Joback Method
cpg	512.08	J/molxK	686.03	Joback Method
cpg	496.24	J/molxK	652.14	Joback Method
cpg	479.47	J/molxK	618.26	Joback Method
cpg	461.73	J/molxK	584.38	Joback Method
cpg	541.12	J/molxK	753.79	Joback Method
dvisc	0.0001548	Paxs	550.50	Joback Method
dvisc	0.0002088	Paxs	501.50	Joback Method
dvisc	0.0003005	Paxs	452.49	Joback Method
dvisc	0.0004725	Paxs	403.49	Joback Method
dvisc	0.0008420	Paxs	354.49	Joback Method
dvisc	0.0018062	Paxs	305.48	Joback Method
dvisc	0.0051862	Paxs	256.48	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=C1079965&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1079965&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>

## 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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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