

# 1,4-di-isopentylbenzene

<b>Inchi:</b>	InChI=1S/C16H26/c1-13(2)5-7-15-9-11-16(12-10-15)8-6-14(3)4/h9-14H,5-8H2,1-4H3
<b>InchiKey:</b>	XKBRARIYUCPYSS-UHFFFAOYSA-N
<b>Formula:</b>	C16H26
<b>SMILES:</b>	CC(C)CCc1ccc(CCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	218.38

## Physical Properties

Property code	Value	Unit	Source
gf	181.74	kJ/mol	Joback Method
hf	-159.07	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.864		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
tb	596.26	K	Joback Method
tc	793.83	K	Joback Method
tf	279.02	K	Joback Method
vc	0.811	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/molxK	596.26	Joback Method
cpg	565.57	J/molxK	629.19	Joback Method
cpg	584.20	J/molxK	662.12	Joback Method
cpg	601.82	J/molxK	695.05	Joback Method
cpg	618.49	J/molxK	727.97	Joback Method
cpg	634.22	J/molxK	760.90	Joback Method
cpg	649.07	J/molxK	793.83	Joback Method
dvisc	0.0046147	Paxs	279.02	Joback Method

dvisc	0.0015822	Paxs	331.89	Joback Method
dvisc	0.0007280	Paxs	384.77	Joback Method
dvisc	0.0004041	Paxs	437.64	Joback Method
dvisc	0.0002546	Paxs	490.51	Joback Method
dvisc	0.0001756	Paxs	543.39	Joback Method
dvisc	0.0001293	Paxs	596.26	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R200781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R200781&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices
<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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