

# 4,4'-Diethylbiphenyl

<b>Inchi:</b>	InChI=1S/C16H18/c1-3-13-5-9-15(10-6-13)16-11-7-14(4-2)8-12-16/h5-12H,3-4H2,1-2H3
<b>InchiKey:</b>	UMSGIWAAMHRVQI-UHFFFAOYSA-N
<b>Formula:</b>	C16H18
<b>SMILES:</b>	CCc1ccc(-c2ccc(CC)cc2)cc1
<b>Mol. weight [g/mol]:</b>	210.31
<b>CAS:</b>	13049-40-6

## Physical Properties

Property code	Value	Unit	Source
gf	289.40	kJ/mol	Joback Method
hf	76.55	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.478		Crippen Method
mvol	188.780	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
tb	586.30 ± 4.00	K	NIST Webbook
tc	860.73	K	Joback Method
tf	356.00 ± 5.00	K	NIST Webbook
tf	354.00 ± 4.00	K	NIST Webbook
tf	353.00 ± 3.00	K	NIST Webbook
vc	0.716	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.73	J/mol×K	628.80	Joback Method
cpg	489.89	J/mol×K	667.45	Joback Method
cpg	506.82	J/mol×K	706.11	Joback Method
cpg	522.58	J/mol×K	744.76	Joback Method
cpg	537.22	J/mol×K	783.42	Joback Method
cpg	550.82	J/mol×K	822.07	Joback Method
cpg	563.43	J/mol×K	860.73	Joback Method

dvisc	0.0014473	Paxs	347.96	Joback Method
dvisc	0.0007888	Paxs	394.77	Joback Method
dvisc	0.0004889	Paxs	441.57	Joback Method
dvisc	0.0003321	Paxs	488.38	Joback Method
dvisc	0.0002414	Paxs	535.19	Joback Method
dvisc	0.0001847	Paxs	581.99	Joback Method
dvisc	0.0001471	Paxs	628.80	Joback Method

## Sources

<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=C13049406&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13049406&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>

## 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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