

# Toluene, 3,4-bis(benzyloxy)-

<b>Inchi:</b>	InChI=1S/C21H20O2/c1-17-12-13-20(22-15-18-8-4-2-5-9-18)21(14-17)23-16-19-10-6-3-7
<b>InchiKey:</b>	JQAYGWDEFVAVMCJ-UHFFFAOYSA-N
<b>Formula:</b>	C21H20O2
<b>SMILES:</b>	<chem>Cc1ccc(OCc2ccccc2)c(OCc2ccccc2)c1</chem>
<b>Mol. weight [g/mol]:</b>	304.38
<b>CAS:</b>	4790-00-5

## Physical Properties

Property code	Value	Unit	Source
gf	233.91	kJ/mol	Joback Method
hf	-54.56	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.153		Crippen Method
mvol	247.210	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
tb	814.72	K	Joback Method
tc	1059.61	K	Joback Method
tf	475.19	K	Joback Method
vc	0.923	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.37	J/molxK	814.72	Joback Method
cpg	730.22	J/molxK	855.53	Joback Method
cpg	745.55	J/molxK	896.35	Joback Method
cpg	759.42	J/molxK	937.16	Joback Method
cpg	771.90	J/molxK	977.98	Joback Method
cpg	783.06	J/molxK	1018.79	Joback Method
cpg	792.94	J/molxK	1059.61	Joback Method
dvisc	0.0004930	Paxs	475.19	Joback Method
dvisc	0.0002798	Paxs	531.78	Joback Method

dvisc	0.0001770	Paxs	588.37	Joback Method
dvisc	0.0001214	Paxs	644.96	Joback Method
dvisc	0.0000885	Paxs	701.54	Joback Method
dvisc	0.0000676	Paxs	758.13	Joback Method
dvisc	0.0000536	Paxs	814.72	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C4790005&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4790005&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>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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