

# p-Toluic acid, benzyl ester

<b>Other names:</b>	Benzyl 4-methylbenzoate
<b>Inchi:</b>	InChI=1S/C15H14O2/c1-12-7-9-14(10-8-12)15(16)17-11-13-5-3-2-4-6-13/h2-10H,11H2,1
<b>InchiKey:</b>	LNXGEZSXCGDUSD-UHFFFAOYSA-N
<b>Formula:</b>	C15H14O2
<b>SMILES:</b>	<chem>Cc1ccc(C(=O)OCc2ccccc2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	226.27
<b>CAS:</b>	5467-99-2

## Physical Properties

Property code	Value	Unit	Source
gf	56.69	kJ/mol	Joback Method
hf	-136.14	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.352		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1881.40		NIST Webbook
rinpol	1884.80		NIST Webbook
rinpol	1881.40		NIST Webbook
tb	677.23	K	Joback Method
tc	915.77	K	Joback Method
tf	396.33	K	Joback Method
vc	0.683	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.84	J/molxK	677.23	Joback Method
cpg	481.42	J/molxK	716.99	Joback Method
cpg	495.81	J/molxK	756.74	Joback Method
cpg	509.05	J/molxK	796.50	Joback Method
cpg	521.19	J/molxK	836.25	Joback Method

cpg	532.27	J/mol×K	876.01	Joback Method
cpg	542.35	J/mol×K	915.77	Joback Method
dvisc	0.0012300	Paxs	396.33	Joback Method
dvisc	0.0007015	Paxs	443.15	Joback Method
dvisc	0.0004454	Paxs	489.96	Joback Method
dvisc	0.0003061	Paxs	536.78	Joback Method
dvisc	0.0002234	Paxs	583.60	Joback Method
dvisc	0.0001709	Paxs	630.41	Joback Method
dvisc	0.0001356	Paxs	677.23	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=C5467992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5467992&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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