

# p-Toluic acid, 3-tetradecyl ester

<b>Other names:</b>	p-Toluylic acid, 3-tetradecyl ester
<b>Inchi:</b>	InChI=1S/C22H36O2/c1-4-6-7-8-9-10-11-12-13-14-21(5-2)24-22(23)20-17-15-19(3)16-18
<b>InchiKey:</b>	KBZKQLNJDBQUGZ-UHFFFAOYSA-N
<b>Formula:</b>	C22H36O2
<b>SMILES:</b>	CCCCCCCCCCCC(CC)OC(=O)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	332.52

## Physical Properties

Property code	Value	Unit	Source
gf	0.78	kJ/mol	Joback Method
hf	-522.43	kJ/mol	Joback Method
hfus	45.65	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.851		Crippen Method
mvol	304.520	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	810.27	K	Joback Method
tc	1004.22	K	Joback Method
tf	433.80	K	Joback Method
vc	1.177	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.66	J/mol×K	810.27	Joback Method
cpg	964.50	J/mol×K	842.59	Joback Method
cpg	982.20	J/mol×K	874.92	Joback Method
cpg	998.82	J/mol×K	907.24	Joback Method
cpg	1014.39	J/mol×K	939.57	Joback Method
cpg	1028.95	J/mol×K	971.89	Joback Method
cpg	1042.54	J/mol×K	1004.22	Joback Method

dvisc	0.0010196	Paxs	433.80	Joback Method
dvisc	0.0004550	Paxs	496.55	Joback Method
dvisc	0.0002433	Paxs	559.29	Joback Method
dvisc	0.0001476	Paxs	622.03	Joback Method
dvisc	0.0000982	Paxs	684.78	Joback Method
dvisc	0.0000699	Paxs	747.52	Joback Method
dvisc	0.0000525	Paxs	810.27	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=U299807&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299807&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>mvol:</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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