

# o-Toluic acid, 2-tetradecyl ester

<b>Other names:</b>	o-Toluylic acid, 2-tetradecyl ester
<b>Inchi:</b>	InChI=1S/C22H36O2/c1-4-5-6-7-8-9-10-11-12-13-17-20(3)24-22(23)21-18-15-14-16-19(2)
<b>InchiKey:</b>	OOMDUBBTCIPRQS-UHFFFAOYSA-N
<b>Formula:</b>	C22H36O2
<b>SMILES:</b>	CCCCCCCCCCCC(C)OC(=O)c1ccccc1C
<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
mcvol	304.520	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2346.00		NIST Webbook
tb	810.27	K	Joback Method
tc	1004.22	K	Joback Method
tf	433.80	K	Joback Method
vc	1.177	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.66	J/molxK	810.27	Joback Method
cpg	1028.95	J/molxK	971.89	Joback Method
cpg	1014.39	J/molxK	939.57	Joback Method
cpg	998.82	J/molxK	907.24	Joback Method
cpg	982.20	J/molxK	874.92	Joback Method
cpg	964.50	J/molxK	842.59	Joback Method
cpg	1042.54	J/molxK	1004.22	Joback Method
dvisc	0.0000525	Paxs	810.27	Joback Method

dvisc	0.0000699	Paxs	747.52	Joback Method
dvisc	0.0000982	Paxs	684.78	Joback Method
dvisc	0.0001476	Paxs	622.03	Joback Method
dvisc	0.0002433	Paxs	559.29	Joback Method
dvisc	0.0004550	Paxs	496.55	Joback Method
dvisc	0.0010196	Paxs	433.80	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299794&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>
<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>

## 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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