

# o-Toluic acid, 4-pentadecyl ester

<b>Other names:</b>	o-Toluylic acid, 4-pentadecyl ester
<b>Inchi:</b>	InChI=1S/C23H38O2/c1-4-6-7-8-9-10-11-12-13-18-21(16-5-2)25-23(24)22-19-15-14-17-2
<b>InchiKey:</b>	CQIOYPLDPXFMMM-UHFFFAOYSA-N
<b>Formula:</b>	C23H38O2
<b>SMILES:</b>	CCCCCCCCCCCC(CCC)OC(=O)c1ccccc1C
<b>Mol. weight [g/mol]:</b>	346.55

## Physical Properties

Property code	Value	Unit	Source
gf	9.20	kJ/mol	Joback Method
hf	-543.07	kJ/mol	Joback Method
hfus	48.24	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.241		Crippen Method
mvol	318.610	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2384.00		NIST Webbook
tb	833.15	K	Joback Method
tc	1028.23	K	Joback Method
tf	445.07	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.47	J/molxK	833.15	Joback Method
cpg	1090.56	J/molxK	995.71	Joback Method
cpg	1075.90	J/molxK	963.20	Joback Method
cpg	1060.20	J/molxK	930.69	Joback Method
cpg	1043.42	J/molxK	898.18	Joback Method
cpg	1025.53	J/molxK	865.66	Joback Method
cpg	1104.22	J/molxK	1028.23	Joback Method
dvisc	0.0000457	Paxs	833.15	Joback Method

dvisc	0.0000610	Paxs	768.47	Joback Method
dvisc	0.0000859	Paxs	703.79	Joback Method
dvisc	0.0001297	Paxs	639.11	Joback Method
dvisc	0.0002149	Paxs	574.43	Joback Method
dvisc	0.0004045	Paxs	509.75	Joback Method
dvisc	0.0009154	Paxs	445.07	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=U299800&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299800&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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