

# m-Toluic acid, 4-hexadecyl ester

<b>Other names:</b>	m-toluylic acid, 4-hexadecyl ester
<b>Inchi:</b>	InChI=1S/C24H40O2/c1-4-6-7-8-9-10-11-12-13-14-19-23(16-5-2)26-24(25)22-18-15-17-2
<b>InchiKey:</b>	CUUFWOWUANSdle-UHFFFAOYSA-N
<b>Formula:</b>	C24H40O2
<b>SMILES:</b>	CCCCCCCCCCCC(CCC)OC(=O)c1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	360.57

## Physical Properties

Property code	Value	Unit	Source
gf	17.62	kJ/mol	Joback Method
hf	-563.71	kJ/mol	Joback Method
hfus	50.83	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	7.632		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2499.90		NIST Webbook
tb	856.03	K	Joback Method
tc	1052.96	K	Joback Method
tf	456.34	K	Joback Method
vc	1.290	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.02	J/molxK	856.03	Joback Method
cpg	1087.32	J/molxK	888.85	Joback Method
cpg	1105.41	J/molxK	921.67	Joback Method
cpg	1122.35	J/molxK	954.50	Joback Method
cpg	1138.18	J/molxK	987.32	Joback Method
cpg	1152.93	J/molxK	1020.14	Joback Method
cpg	1166.67	J/molxK	1052.96	Joback Method
dvisc	0.0008185	Paxs	456.34	Joback Method

dvisc	0.0003584	Paxs	522.95	Joback Method
dvisc	0.0001891	Paxs	589.57	Joback Method
dvisc	0.0001136	Paxs	656.18	Joback Method
dvisc	0.0000750	Paxs	722.80	Joback Method
dvisc	0.0000531	Paxs	789.41	Joback Method
dvisc	0.0000397	Paxs	856.03	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=U292239&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292239&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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