

# m-Toluic acid, heptadecyl ester

<b>Other names:</b>	m-toluylic acid, heptadecyl ester
<b>Inchi:</b>	InChI=1S/C25H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-27-25(26)24-20-18-
<b>InchiKey:</b>	GWRNAFAWUNRDOT-UHFFFAOYSA-N
<b>Formula:</b>	C25H42O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	374.60

## Physical Properties

Property code	Value	Unit	Source
gf	28.48	kJ/mol	Joback Method
hf	-579.07	kJ/mol	Joback Method
hfus	56.94	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.023		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2742.20		NIST Webbook
rinpol	2742.20		NIST Webbook
tb	879.35	K	Joback Method
tc	1078.25	K	Joback Method
tf	482.61	K	Joback Method
vc	1.351	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.80	J/molxK	879.35	Joback Method
cpg	1215.57	J/molxK	1045.10	Joback Method
cpg	1200.69	J/molxK	1011.95	Joback Method
cpg	1184.71	J/molxK	978.80	Joback Method
cpg	1167.61	J/molxK	945.65	Joback Method
cpg	1149.32	J/molxK	912.50	Joback Method
cpg	1229.43	J/molxK	1078.25	Joback Method

dvisc	0.0000376	Paxs	879.35	Joback Method
dvisc	0.0000496	Paxs	813.23	Joback Method
dvisc	0.0000689	Paxs	747.10	Joback Method
dvisc	0.0001020	Paxs	680.98	Joback Method
dvisc	0.0001641	Paxs	614.86	Joback Method
dvisc	0.0002964	Paxs	548.73	Joback Method
dvisc	0.0006292	Paxs	482.61	Joback Method

## Sources

<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=U292240&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292240&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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