

# m-Toluic acid, 2-(1-adamantyl)ethyl ester

<b>Other names:</b>	m-toluylic acid, 2-(1-adamantyl)ethyl ester
<b>Inchi:</b>	InChI=1S/C20H26O2/c1-14-3-2-4-18(7-14)19(21)22-6-5-20-11-15-8-16(12-20)10-17(9-15)
<b>InchiKey:</b>	QXDLZKOHACFPPP-UHFFFAOYSA-N
<b>Formula:</b>	C20H26O2
<b>SMILES:</b>	<chem>Cc1cccc(C(=O)OCCC23CC4CC(CC(C4)C2)C3)c1</chem>
<b>Mol. weight [g/mol]:</b>	298.42

## Physical Properties

Property code	Value	Unit	Source
gf	143.33	kJ/mol	Joback Method
hf	-268.73	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.758		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2445.70		NIST Webbook
rinpol	2445.70		NIST Webbook
tb	785.01	K	Joback Method
tc	1017.93	K	Joback Method
tf	496.22	K	Joback Method
vc	0.931	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.45	J/molxK	785.01	Joback Method
cpg	802.52	J/molxK	823.83	Joback Method
cpg	822.82	J/molxK	862.65	Joback Method
cpg	842.60	J/molxK	901.47	Joback Method
cpg	862.09	J/molxK	940.29	Joback Method
cpg	881.54	J/molxK	979.11	Joback Method
cpg	901.21	J/molxK	1017.93	Joback Method

# Sources

<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=U292236&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292236&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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