

# p-Toluic acid, 1-adamantylmethyl ester

<b>Other names:</b>	p-toluylic acid, 1-adamantylmethyl ester
<b>Inchi:</b>	InChI=1S/C19H24O2/c1-13-2-4-17(5-3-13)18(20)21-12-19-9-14-6-15(10-19)8-16(7-14)1
<b>InchiKey:</b>	ACTFIILMCRWJJK-UHFFFAOYSA-N
<b>Formula:</b>	C19H24O2
<b>SMILES:</b>	<chem>Cc1ccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)cc1</chem>
<b>Mol. weight [g/mol]:</b>	284.39

## Physical Properties

Property code	Value	Unit	Source
gf	134.91	kJ/mol	Joback Method
hf	-248.09	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.368		Crippen Method
mcvol	229.670	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2290.80		NIST Webbook
rinpol	2290.80		NIST Webbook
tb	762.13	K	Joback Method
tc	999.19	K	Joback Method
tf	484.95	K	Joback Method
vc	0.875	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.41	J/molxK	762.13	Joback Method
cpg	744.17	J/molxK	801.64	Joback Method
cpg	764.07	J/molxK	841.15	Joback Method
cpg	783.36	J/molxK	880.66	Joback Method
cpg	802.29	J/molxK	920.17	Joback Method
cpg	821.11	J/molxK	959.68	Joback Method
cpg	840.10	J/molxK	999.19	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=U292217&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292217&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.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>

# 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>h vap:</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>r in pol:</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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