

# m-Toluic acid, but-3-yn-2-yl ester

<b>Other names:</b>	m-toluylic acid, but-3-yn-2-yl ester
<b>Inchi:</b>	InChI=1S/C12H12O2/c1-4-10(3)14-12(13)11-7-5-6-9(2)8-11/h1,5-8,10H,2-3H3
<b>InchiKey:</b>	KAOKEECXRDGMGW-UHFFFAOYSA-N
<b>Formula:</b>	C12H12O2
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)c1cccc(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	188.22

## Physical Properties

Property code	Value	Unit	Source
gf	139.65	kJ/mol	Joback Method
hf	-24.13	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.174		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1404.20		NIST Webbook
tb	571.59	K	Joback Method
tc	797.96	K	Joback Method
tf	368.07	K	Joback Method
vc	0.580	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.57	J/mol×K	571.59	Joback Method
cpg	368.54	J/mol×K	609.32	Joback Method
cpg	381.64	J/mol×K	647.05	Joback Method
cpg	393.90	J/mol×K	684.77	Joback Method
cpg	405.34	J/mol×K	722.50	Joback Method
cpg	416.00	J/mol×K	760.23	Joback Method
cpg	425.91	J/mol×K	797.96	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292494&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292494&amp;Units=SI</a>
<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>

# 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>hvpap:</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>rinppl:</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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