

# p-Toluic acid, hex-4-yn-3-yl ester

<b>Other names:</b>	p-toluylic acid, hex-4-yn-3-yl ester
<b>Inchi:</b>	InChI=1S/C14H16O2/c1-4-6-13(5-2)16-14(15)12-9-7-11(3)8-10-12/h7-10,13H,5H2,1-3H3
<b>InchiKey:</b>	TVCDXZNMUSFMLC-UHFFFAOYSA-N
<b>Formula:</b>	C14H16O2
<b>SMILES:</b>	CC#CC(CC)OC(=O)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	216.28

## Physical Properties

Property code	Value	Unit	Source
gf	136.22	kJ/mol	Joback Method
hf	-85.01	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.954		Crippen Method
mvol	183.200	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1685.50		NIST Webbook
tb	636.23	K	Joback Method
tc	864.73	K	Joback Method
tf	449.74	K	Joback Method
vc	0.692	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.85	J/mol×K	636.23	Joback Method
cpg	468.77	J/mol×K	674.31	Joback Method
cpg	483.70	J/mol×K	712.40	Joback Method
cpg	497.67	J/mol×K	750.48	Joback Method
cpg	510.69	J/mol×K	788.57	Joback Method
cpg	522.80	J/mol×K	826.65	Joback Method
cpg	534.01	J/mol×K	864.73	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292504&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292504&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>hvp:</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>rinp:</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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