

# o-Anisic acid, hex-4-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C14H16O3/c1-4-8-11(5-2)17-14(15)12-9-6-7-10-13(12)16-3/h6-7,9-11H,5H2,1
<b>InchiKey:</b>	SCJRVUIAGQRMQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H16O3
<b>SMILES:</b>	CC#CC(CC)OC(=O)c1ccccc1OC
<b>Mol. weight [g/mol]:</b>	232.28

## Physical Properties

Property code	Value	Unit	Source
gf	31.22	kJ/mol	Joback Method
hf	-217.23	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	63.03	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.654		Crippen Method
mcvol	189.070	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinsol	1750.20		NIST Webbook
tb	658.65	K	Joback Method
tc	884.05	K	Joback Method
tf	471.97	K	Joback Method
vc	0.710	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.71	J/mol×K	658.65	Joback Method
cpg	494.28	J/mol×K	696.22	Joback Method
cpg	508.90	J/mol×K	733.78	Joback Method
cpg	522.56	J/mol×K	771.35	Joback Method
cpg	535.28	J/mol×K	808.92	Joback Method
cpg	547.05	J/mol×K	846.48	Joback Method
cpg	557.89	J/mol×K	884.05	Joback Method

# Sources

<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>
<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=U292574&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292574&amp;Units=SI</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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