

# m-Anisic acid, oct-3-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H22O3/c1-4-5-6-7-9-13(2)19-16(17)14-10-8-11-15(12-14)18-3/h7-13H,4-6H
<b>InchiKey:</b>	ILFVQCDACZZNIV-VQHVLOKHSA-N
<b>Formula:</b>	C16H22O3
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	262.34

## Physical Properties

Property code	Value	Unit	Source
gf	-74.52	kJ/mol	Joback Method
hf	-413.59	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.987		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1932.80		NIST Webbook
rinpol	1932.80		NIST Webbook
tb	699.57	K	Joback Method
tc	904.52	K	Joback Method
tf	383.33	K	Joback Method
vc	0.840	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.00	J/molxK	699.57	Joback Method
cpg	622.45	J/molxK	733.73	Joback Method
cpg	637.93	J/molxK	767.89	Joback Method
cpg	652.45	J/molxK	802.04	Joback Method
cpg	666.05	J/molxK	836.20	Joback Method
cpg	678.75	J/molxK	870.36	Joback Method
cpg	690.57	J/molxK	904.52	Joback Method
dvisc	0.0011364	Paxs	383.33	Joback Method

dvisc	0.0005496	Paxs	436.04	Joback Method
dvisc	0.0003109	Paxs	488.74	Joback Method
dvisc	0.0001965	Paxs	541.45	Joback Method
dvisc	0.0001347	Paxs	594.16	Joback Method
dvisc	0.0000982	Paxs	646.86	Joback Method
dvisc	0.0000751	Paxs	699.57	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292595&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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