

# o-Anisic acid, 4-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C15H14O4/c1-17-11-7-9-12(10-8-11)19-15(16)13-5-3-4-6-14(13)18-2/h3-10H,1
<b>InchiKey:</b>	PNFGKOBYWQFVKR-UHFFFAOYSA-N
<b>Formula:</b>	C15H14O4
<b>SMILES:</b>	COc1ccc(OC(=O)c2ccccc2OC)cc1
<b>Mol. weight [g/mol]:</b>	258.27

## Physical Properties

Property code	Value	Unit	Source
gf	-162.94	kJ/mol	Joback Method
hf	-412.05	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.923		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinsol	2127.00		NIST Webbook
tb	727.05	K	Joback Method
tc	959.54	K	Joback Method
tf	453.31	K	Joback Method
vc	0.720	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.43	J/molxK	727.05	Joback Method
cpg	530.98	J/molxK	765.80	Joback Method
cpg	544.39	J/molxK	804.55	Joback Method
cpg	556.66	J/molxK	843.29	Joback Method
cpg	567.78	J/molxK	882.04	Joback Method
cpg	577.76	J/molxK	920.79	Joback Method
cpg	586.59	J/molxK	959.54	Joback Method
dvisc	0.0005592	Paxs	453.31	Joback Method
dvisc	0.0003516	Paxs	498.93	Joback Method

dvisc	0.0002390	Paxs	544.56	Joback Method
dvisc	0.0001724	Paxs	590.18	Joback Method
dvisc	0.0001304	Paxs	635.80	Joback Method
dvisc	0.0001023	Paxs	681.43	Joback Method
dvisc	0.0000828	Paxs	727.05	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=U307792&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307792&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## 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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