

# m-Anisic acid, 3,4-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H10Cl2O3/c1-18-10-4-2-3-9(7-10)14(17)19-11-5-6-12(15)13(16)8-11/h2-8
<b>InchiKey:</b>	NKZQQSMRSOXSET-UHFFFAOYSA-N
<b>Formula:</b>	C14H10Cl2O3
<b>SMILES:</b>	COc1cccc(C(=O)Oc2ccc(Cl)c(Cl)c2)c1
<b>Mol. weight [g/mol]:</b>	297.13

## Physical Properties

Property code	Value	Unit	Source
gf	-99.85	kJ/mol	Joback Method
hf	-302.14	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.221		Crippen Method
mcvol	198.390	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	761.59	K	Joback Method
tc	1007.60	K	Joback Method
tf	492.17	K	Joback Method
vc	0.744	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/molxK	761.59	Joback Method
cpg	495.91	J/molxK	802.59	Joback Method
cpg	506.68	J/molxK	843.59	Joback Method
cpg	516.38	J/molxK	884.59	Joback Method
cpg	525.01	J/molxK	925.60	Joback Method
cpg	532.59	J/molxK	966.60	Joback Method
cpg	539.12	J/molxK	1007.60	Joback Method
dvisc	0.0005499	Paxs	492.17	Joback Method

dvisc	0.0003674	Paxs	537.07	Joback Method
dvisc	0.0002612	Paxs	581.98	Joback Method
dvisc	0.0001950	Paxs	626.88	Joback Method
dvisc	0.0001514	Paxs	671.78	Joback Method
dvisc	0.0001213	Paxs	716.69	Joback Method
dvisc	0.0000998	Paxs	761.59	Joback Method

## Sources

<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=U307803&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307803&amp;Units=SI</a>
<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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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