

# Benzoic acid, 3,4-dimethyl-, methyl ester

<b>Other names:</b>	3,4-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> -CO <sub>2</sub> CH <sub>3</sub> Methyl 3,4-dimethylbenzoate
<b>Inchi:</b>	InChI=1S/C10H12O2/c1-7-4-5-9(6-8(7)2)10(11)12-3/h4-6H,1-3H3
<b>InchiKey:</b>	PTSSKYUSCIALKU-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O2
<b>SMILES:</b>	COC(=O)c1ccc(C)c(C)c1
<b>Mol. weight [g/mol]:</b>	164.20
<b>CAS:</b>	38404-42-1

## Physical Properties

Property code	Value	Unit	Source
affp	868.50	kJ/mol	NIST Webbook
basg	837.50	kJ/mol	NIST Webbook
gf	-107.45	kJ/mol	Joback Method
hf	-280.94	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.090		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	231.10		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1352.00		NIST Webbook
tb	541.13	K	Joback Method
tc	756.04	K	Joback Method
tf	326.08	K	Joback Method
vc	0.511	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.97	J/molxK	541.13	Joback Method

cpg	312.92	J/molxK	576.95	Joback Method
cpg	325.22	J/molxK	612.77	Joback Method
cpg	336.88	J/molxK	648.58	Joback Method
cpg	347.89	J/molxK	684.40	Joback Method
cpg	358.27	J/molxK	720.22	Joback Method
cpg	368.03	J/molxK	756.04	Joback Method
dvisc	0.0013513	Paxs	326.08	Joback Method
dvisc	0.0008436	Paxs	361.92	Joback Method
dvisc	0.0005733	Paxs	397.76	Joback Method
dvisc	0.0004153	Paxs	433.61	Joback Method
dvisc	0.0003161	Paxs	469.45	Joback Method
dvisc	0.0002500	Paxs	505.29	Joback Method
dvisc	0.0002040	Paxs	541.13	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=C38404421&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38404421&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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