

# Phenol, 3-(1,1-dimethylethyl)-4-methoxy-

<b>Other names:</b>	Phenol, 3-tert-butyl-4-methoxy- 3-tert-Butylated hydroxyanisole 3-tert-Butyl-4-methoxyphenol 2-tert-Butyl-4-hydroxy anisole 4-Methoxy-3-tert-butylphenol
<b>Inchi:</b>	InChI=1S/C11H16O2/c1-11(2,3)9-7-8(12)5-6-10(9)13-4/h5-7,12H,1-4H3
<b>InchiKey:</b>	IMOYOUUMVYICGCA-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O2
<b>SMILES:</b>	COc1ccc(O)cc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	180.24
<b>CAS:</b>	88-32-4

## Physical Properties

Property code	Value	Unit	Source
gf	-112.26	kJ/mol	Joback Method
hf	-363.59	kJ/mol	Joback Method
hfus	17.46	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.698		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	582.55	K	Joback Method
tc	809.07	K	Joback Method
tf	389.04	K	Joback Method
vc	0.516	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.33	J/molxK	582.55	Joback Method
cpg	400.12	J/molxK	620.30	Joback Method

cpg	413.90	J/mol×K	658.06	Joback Method
cpg	426.77	J/mol×K	695.81	Joback Method
cpg	438.81	J/mol×K	733.56	Joback Method
cpg	450.10	J/mol×K	771.32	Joback Method
cpg	460.74	J/mol×K	809.07	Joback Method
dvisc	0.0010688	Paxs	389.04	Joback Method
dvisc	0.0004674	Paxs	421.29	Joback Method
dvisc	0.0002299	Paxs	453.54	Joback Method
dvisc	0.0001242	Paxs	485.79	Joback Method
dvisc	0.0000725	Paxs	518.05	Joback Method
dvisc	0.0000451	Paxs	550.30	Joback Method
dvisc	0.0000295	Paxs	582.55	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=C88324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88324&amp;Units=SI</a>
<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>

## 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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