

# m-(tert-Butyl)anisole

<b>Inchi:</b>	InChI=1S/C11H16O/c1-11(2,3)9-6-5-7-10(8-9)12-4/h5-8H,1-4H3
<b>InchiKey:</b>	IPGSPXKLIPOGON-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O
<b>SMILES:</b>	COc1cccc(C(C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	164.24

## Physical Properties

Property code	Value	Unit	Source
gf	42.36	kJ/mol	Joback Method
hf	-186.28	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	44.13	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.993		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	501.93	K	Joback Method
tc	716.64	K	Joback Method
tf	277.32	K	Joback Method
vc	0.550	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.05	J/molxK	501.93	Joback Method
cpg	345.56	J/molxK	537.72	Joback Method
cpg	361.09	J/molxK	573.50	Joback Method
cpg	375.70	J/molxK	609.29	Joback Method
cpg	389.41	J/molxK	645.07	Joback Method
cpg	402.27	J/molxK	680.86	Joback Method
cpg	414.31	J/molxK	716.64	Joback Method
dvisc	0.0026267	Paxs	277.32	Joback Method

dvisc	0.0012719	Paxs	314.75	Joback Method
dvisc	0.0007186	Paxs	352.19	Joback Method
dvisc	0.0004530	Paxs	389.62	Joback Method
dvisc	0.0003097	Paxs	427.06	Joback Method
dvisc	0.0002251	Paxs	464.50	Joback Method
dvisc	0.0001715	Paxs	501.93	Joback Method

## Sources

<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=R543494&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R543494&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>

## 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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