

# 4-tert-Butylcatechol, dimethyl ether

<b>Inchi:</b>	InChI=1S/C12H18O2/c1-12(2,3)9-6-7-10(13-4)11(8-9)14-5/h6-8H,1-5H3
<b>InchiKey:</b>	FSWSUKGIUZLXKK-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O2
<b>SMILES:</b>	COc1ccc(C(C)(C)C)cc1OC
<b>Mol. weight [g/mol]:</b>	194.27

## Physical Properties

Property code	Value	Unit	Source
gf	-63.85	kJ/mol	Joback Method
hf	-350.61	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	49.43	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.001		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1430.10		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	552.21	K	Joback Method
tc	762.44	K	Joback Method
tf	323.34	K	Joback Method
vc	0.625	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.85	J/molxK	552.21	Joback Method
cpg	475.86	J/molxK	727.40	Joback Method
cpg	462.72	J/molxK	692.36	Joback Method
cpg	448.77	J/molxK	657.32	Joback Method
cpg	433.99	J/molxK	622.29	Joback Method
cpg	418.35	J/molxK	587.25	Joback Method
cpg	488.20	J/molxK	762.44	Joback Method
dvisc	0.0001232	Paxs	552.21	Joback Method

dvisc	0.0001581	Paxs	514.07	Joback Method
dvisc	0.0002111	Paxs	475.92	Joback Method
dvisc	0.0002966	Paxs	437.78	Joback Method
dvisc	0.0004445	Paxs	399.63	Joback Method
dvisc	0.0007257	Paxs	361.49	Joback Method
dvisc	0.0013298	Paxs	323.34	Joback Method

## Sources

<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>
<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=U352796&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352796&amp;Units=SI</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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