

# 2,6-Ditert-buthyl-4-hydroxy toluene

<b>Other names:</b>	2,6-bis(1,1-dimethylethyl)-4-methylphenol 2,6-bis(tert-butyl)-4-methylphenol 2,6-di-tert-butyl-4-hydroxytoluene 2,6-di-tert-butyl-4-methylphenol 2,6-di-tert-butyl-p-cresol 2,6-di-tert-butyl-p-methylphenol 2,6-di-tert-butylmethylphenol 2,6-tert-butyl-4-methylphenol 3,5-di-tert-butyl-4-hydroxytoluene 4-hydroxy-3,5-di-tert-butyltoluene 4-methyl-2,6-di-tert-butylphenol DBPC advastab 401 agidol alkofen BP antage BHT antioxidant 264 butylated hydroxytoluene chemanox 11 dibunol dibutylated hydroxytoluene ionol ionole phenol, 1,6-bis(1,1-dimethylethyl)-4-methyl-
<b>Inchi:</b>	InChI=1S/C15H24O/c1-10-12(14(2,3)4)8-11(16)9-13(10)15(5,6)7/h8-9,16H,1-7H3
<b>InchiKey:</b>	SMNGQGWPVVORF-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>Cc1c(C(C)(C)C)cc(O)cc1C(C)(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	19.63	kJ/mol	Joback Method
hf	-334.15	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	63.01	kJ/mol	Joback Method

log10ws	-4.12		Crippen Method
logp	4.296		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinsol	1519.00		NIST Webbook
tb	653.40	K	Joback Method
tc	880.13	K	Joback Method
tf	343.15	K	Liquid pharmaceuticals formulation by eutectic formation
vc	0.712	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.55	J/molxK	653.40	Joback Method
cpg	580.43	J/molxK	691.19	Joback Method
cpg	597.12	J/molxK	728.98	Joback Method
cpg	612.75	J/molxK	766.77	Joback Method
cpg	627.45	J/molxK	804.56	Joback Method
cpg	641.37	J/molxK	842.35	Joback Method
cpg	654.63	J/molxK	880.13	Joback Method
dvisc	0.0006069	Paxs	426.83	Joback Method
dvisc	0.0002505	Paxs	464.59	Joback Method
dvisc	0.0001181	Paxs	502.35	Joback Method
dvisc	0.0000618	Paxs	540.12	Joback Method
dvisc	0.0000352	Paxs	577.88	Joback Method
dvisc	0.0000215	Paxs	615.64	Joback Method
dvisc	0.0000139	Paxs	653.40	Joback Method

## Sources

Probing effect of lipophilic butylated hydroxytoluene on anionic surfactant based pharmaceutical formulation by eutectic formation: Thermodynamic and spectroscopic study.

<https://www.doi.org/10.1016/j.fluid.2014.03.032>

McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2017.05.009>

NIST Webbook:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R417300&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# 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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