

# Benzenethiol, 4-(1,1-dimethylethyl)-2-methyl-

<b>Other names:</b>	o-Toluenethiol, 4-tert-butyl- 4-tert-Butyl-o-Thiocresol 4-tert-Butyl-2-Methylthiophenol
<b>Inchi:</b>	InChI=1S/C11H16S/c1-8-7-9(11(2,3)4)5-6-10(8)12/h5-7,12H,1-4H3
<b>InchiKey:</b>	DUZJXKYBSMFDIU-UHFFFAOYSA-N
<b>Formula:</b>	C11H16S
<b>SMILES:</b>	<chem>Cc1cc(C(C)(C)C)ccc1S</chem>
<b>Mol. weight [g/mol]:</b>	180.31
<b>CAS:</b>	15570-10-2

## Physical Properties

Property code	Value	Unit	Source
gf	167.12	kJ/mol	Joback Method
hf	-27.05	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.581		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	547.35	K	Joback Method
tc	787.39	K	Joback Method
tf	304.07	K	Joback Method
vc	0.587	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.43	J/mol×K	547.35	Joback Method
cpg	373.05	J/mol×K	587.36	Joback Method
cpg	388.52	J/mol×K	627.36	Joback Method
cpg	402.90	J/mol×K	667.37	Joback Method
cpg	416.25	J/mol×K	707.38	Joback Method
cpg	428.64	J/mol×K	747.38	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=C15570102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15570102&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>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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