

# 2-tert-Butylthiophenol

<b>Inchi:</b>	InChI=1S/C10H14S/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7,11H,1-3H3
<b>InchiKey:</b>	BKMGLHQPYECKPO-UHFFFAOYSA-N
<b>Formula:</b>	C10H14S
<b>SMILES:</b>	CC(C)(C)c1ccccc1S
<b>Mol. weight [g/mol]:</b>	166.28
<b>CAS:</b>	19728-41-7

## Physical Properties

Property code	Value	Unit	Source
gf	168.33	kJ/mol	Joback Method
hf	5.06	kJ/mol	Joback Method
hfus	11.94	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.273		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	519.49	K	Joback Method
tc	763.23	K	Joback Method
tf	280.28	K	Joback Method
vc	0.530	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.71	J/mol×K	519.49	Joback Method
cpg	326.90	J/mol×K	560.11	Joback Method
cpg	341.88	J/mol×K	600.74	Joback Method
cpg	355.73	J/mol×K	641.36	Joback Method
cpg	368.52	J/mol×K	681.98	Joback Method
cpg	380.32	J/mol×K	722.61	Joback Method
cpg	391.22	J/mol×K	763.23	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=C19728417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19728417&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>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>h vap:</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>m cvol:</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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