

# 6-Thymolsulfonic acid

<b>Other names:</b>	5-hydroxy-p-cymene-2-sulphonic acid
<b>Inchi:</b>	InChI=1S/C10H14O4S/c1-6(2)8-5-10(15(12,13)14)7(3)4-9(8)11/h4-6,11H,1-3H3,(H,12,13)
<b>InchiKey:</b>	LYWNNXMNOSKLHY-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O4S
<b>SMILES:</b>	<chem>Cc1cc(O)c(C(C)C)cc1S(=O)(=O)O</chem>
<b>Mol. weight [g/mol]:</b>	230.28
<b>CAS:</b>	96-68-4

## Physical Properties

Property code	Value	Unit	Source
gf	-635.95	kJ/mol	Joback Method
hf	-824.31	kJ/mol	Joback Method
hfus	32.64	kJ/mol	Joback Method
hvap	89.39	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.071		Crippen Method
mcvol	167.830	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	684.98	K	Joback Method
tc	887.24	K	Joback Method
tf	450.02	K	Joback Method
vc	0.593	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.69	J/molxK	684.98	Joback Method
cpg	452.61	J/molxK	718.69	Joback Method
cpg	462.86	J/molxK	752.40	Joback Method
cpg	472.49	J/molxK	786.11	Joback Method
cpg	481.54	J/molxK	819.82	Joback Method
cpg	490.03	J/molxK	853.53	Joback Method
cpg	498.02	J/molxK	887.24	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C96684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96684&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>
<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>

# 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>hvp:</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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