

# 4-t-Butylbenzenesulfonyl chloride

<b>Inchi:</b>	InChI=1S/C10H13ClO2S/c1-10(2,3)8-4-6-9(7-5-8)14(11,12)13/h4-7H,1-3H3
<b>InchiKey:</b>	YEZADZMMVHWFYIY-UHFFFAOYSA-N
<b>Formula:</b>	C10H13ClO2S
<b>SMILES:</b>	CC(C)(C)c1ccc(S(=O)(=O)Cl)cc1
<b>Mol. weight [g/mol]:</b>	232.73
<b>CAS:</b>	15084-51-2

## Physical Properties

Property code	Value	Unit	Source
gf	-341.53	kJ/mol	Joback Method
hf	-502.51	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.912		Crippen Method
mcvol	168.330	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	541.84	K	Joback Method
tc	759.20	K	Joback Method
tf	312.30	K	Joback Method
vc	0.651	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.44	J/molxK	541.84	Joback Method
cpg	383.51	J/molxK	578.07	Joback Method
cpg	397.55	J/molxK	614.29	Joback Method
cpg	410.60	J/molxK	650.52	Joback Method
cpg	422.69	J/molxK	686.74	Joback Method
cpg	433.87	J/molxK	722.97	Joback Method
cpg	444.15	J/molxK	759.20	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15084512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15084512&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>mccvol:</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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