

# 6-Methoxy-m-toluenesulfonyl chloride

<b>Inchi:</b>	InChI=1S/C8H9ClO3S/c1-6-3-4-7(12-2)8(5-6)13(9,10)11/h3-5H,1-2H3
<b>InchiKey:</b>	BJYNYQGJTZULJI-UHFFFAOYSA-N
<b>Formula:</b>	C8H9ClO3S
<b>SMILES:</b>	COc1ccc(C)cc1S(=O)(=O)Cl
<b>Mol. weight [g/mol]:</b>	220.67
<b>CAS:</b>	88040-86-2

## Physical Properties

Property code	Value	Unit	Source
gf	-475.84	kJ/mol	Joback Method
hf	-596.17	kJ/mol	Joback Method
hfus	26.50	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.931		Crippen Method
mcvol	146.020	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	526.71	K	Joback Method
tc	736.61	K	Joback Method
tf	322.09	K	Joback Method
vc	0.569	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.55	J/mol×K	526.71	Joback Method
cpg	310.22	J/mol×K	561.69	Joback Method
cpg	321.31	J/mol×K	596.68	Joback Method
cpg	331.81	J/mol×K	631.66	Joback Method
cpg	341.72	J/mol×K	666.64	Joback Method
cpg	351.00	J/mol×K	701.63	Joback Method
cpg	359.66	J/mol×K	736.61	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C88040862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88040862&amp;Units=SI</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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