

# p-Tolyl propadienyl sulphone

**Inchi:** InChI=1S/C10H10O2S/c1-3-8-13(11,12)10-6-4-9(2)5-7-10/h4-8H,1H2,2H3  
**InchiKey:** XKGAKLCWOYKBBO-UHFFFAOYSA-N  
**Formula:** C10H10O2S  
**SMILES:** C=C=CS(=O)(=O)c1ccc(C)cc1  
**Mol. weight [g/mol]:** 194.25  
**CAS:** 16192-08-8

## Physical Properties

Property code	Value	Unit	Source
chs	-5821.00 ± 3.80	kJ/mol	NIST Webbook
gf	-116.32	kJ/mol	Joback Method
hf	-32.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-145.30 ± 4.00	kJ/mol	NIST Webbook
hfus	27.54	kJ/mol	Joback Method
hvap	59.19	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.067		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	507.59	K	Joback Method
tc	723.67	K	Joback Method
tf	284.71	K	Joback Method
vc	0.575	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.36	J/molxK	507.59	Joback Method
cpg	316.97	J/molxK	543.60	Joback Method
cpg	329.84	J/molxK	579.62	Joback Method
cpg	341.96	J/molxK	615.63	Joback Method
cpg	353.35	J/molxK	651.64	Joback Method
cpg	363.99	J/molxK	687.66	Joback Method
cpg	373.90	J/molxK	723.67	Joback Method

# Sources

<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=C16192088&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16192088&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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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