

# 2-Methyl-2-p-toluenesulfonylamino-1,3-propanediol acetate p-toluenesulfonate

InChI: CC(=O)OCC(C)(COS(=O)(=O)c1ccc(C)cc1)NS(=O)(=O)c1ccc(C)cc1  
InChIKey: IFERCIXUYCPJIU-UHFFFAOYSA-N

Formula: C<sub>20</sub>H<sub>25</sub>NO<sub>7</sub>S<sub>2</sub>

SMILES: CC(=O)OCC(C)(COS(=O)(=O)c1ccc(C)cc1)NS(=O)(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 455.55

## Physical Properties

Property code	Value	Unit	Source
gf	-860.69	kJ/mol	Joback Method
hf	-1245.01	kJ/mol	Joback Method
hfus	59.28	kJ/mol	Joback Method
hvap	119.97	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.309		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	961.53	K	Joback Method
tc	1185.72	K	Joback Method
tf	619.63	K	Joback Method
vc	1.258	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.05	J/mol×K	961.53	Joback Method
cpg	1010.57	J/mol×K	998.90	Joback Method
cpg	1019.29	J/mol×K	1036.26	Joback Method
cpg	1026.22	J/mol×K	1073.63	Joback Method
cpg	1031.40	J/mol×K	1110.99	Joback Method
cpg	1034.83	J/mol×K	1148.36	Joback Method
cpg	1036.55	J/mol×K	1185.72	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004575&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004575&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>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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