

# 3-Amino-p-toluene sulfonic acid

<b>Inchi:</b>	InChI=1S/C7H9NO3S/c1-5-2-3-7(6(8)4-5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)
<b>InchiKey:</b>	FJHGMUDVUAXUEK-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO3S
<b>SMILES:</b>	<chem>Cc1ccc(S(=O)(=O)O)c(N)c1</chem>
<b>Mol. weight [g/mol]:</b>	187.22

## Physical Properties

Property code	Value	Unit	Source
gf	-437.70	kJ/mol	Joback Method
hf	-546.01	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.824		Crippen Method
mvol	129.670	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	608.69	K	Joback Method
tc	813.58	K	Joback Method
tf	402.75	K	Joback Method
vc	0.493	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.73	J/mol×K	608.69	Joback Method
cpg	315.24	J/mol×K	642.84	Joback Method
cpg	324.16	J/mol×K	676.99	Joback Method
cpg	332.50	J/mol×K	711.14	Joback Method
cpg	340.25	J/mol×K	745.28	Joback Method
cpg	347.41	J/mol×K	779.43	Joback Method
cpg	354.00	J/mol×K	813.58	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=B6001362&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001362&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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