

# P-toluenesulfonamide, n-(2-cyanoethyl)-

Inchi:	InChI=1S/C10H12N2O2S/c1-9-3-5-10(6-4-9)15(13,14)12-8-2-7-11/h3-6,12H,2,8H2,1H3
InchiKey:	WAUWKQNTCJXJMA-UHFFFAOYSA-N
Formula:	C10H12N2O2S
SMILES:	Cc1ccc(S(=O)(=O)NCCC#N)cc1
Mol. weight [g/mol]:	224.28
CAS:	2619-22-9

## Physical Properties

Property code	Value	Unit	Source
gf	-109.87	kJ/mol	Joback Method
hf	-259.67	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	76.34	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.187		Crippen Method
mcvol	167.450	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	659.89	K	Joback Method
tc	874.60	K	Joback Method
tf	397.61	K	Joback Method
vc	0.674	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.91	J/molxK	659.89	Joback Method
cpg	426.96	J/molxK	695.67	Joback Method
cpg	438.15	J/molxK	731.46	Joback Method
cpg	448.50	J/molxK	767.24	Joback Method
cpg	458.03	J/molxK	803.03	Joback Method
cpg	466.74	J/molxK	838.81	Joback Method
cpg	474.65	J/molxK	874.60	Joback Method

# Sources

<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=C2619229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2619229&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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>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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