

p-Toluenesulfonylacetonitrile

Other names:	p-Tolylsulfonylacetonitrile 4-Toluenesulfonylacetonitrile Acetonitrile, [(4-methylphenyl)sulfonyl]- p-Toluenesulphonylacetonitrile tosylacetonitrile
Inchi:	InChI=1S/C9H9NO2S/c1-8-2-4-9(5-3-8)13(11,12)7-6-10/h2-5H,7H2,1H3
InchiKey:	BBNNLJMGPASZPD-UHFFFAOYSA-N
Formula:	C9H9NO2S
SMILES:	<chem>Cc1ccc(S(=O)(=O)CC#N)cc1</chem>
Mol. weight [g/mol]:	195.24
CAS:	5697-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-207.68	kJ/mol	Joback Method
hf	-292.50	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	67.68	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.292		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	586.84	K	Joback Method
tc	806.10	K	Joback Method
tf	333.68	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.22	J/molxK	586.84	Joback Method
cpg	331.73	J/molxK	623.38	Joback Method
cpg	342.49	J/molxK	659.93	Joback Method
cpg	352.49	J/molxK	696.47	Joback Method

cpg	361.76	J/mol×K	733.01	Joback Method
cpg	370.30	J/mol×K	769.55	Joback Method
cpg	378.12	J/mol×K	806.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5697449&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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