P-toluenesulfonamide, 3-chloro-

Inchi: InChI=1S/C7H8ClNO2S/c1-5-2-3-6(4-7(5)8)12(9,10)11/h2-4H,1H3,(H2,9,10,11)
InchiKey: YAUUWNCFVUUNCM-UHFFFAOYSA-N
Formula: C7H8ClNO2S
SMILES: Cc1ccc(S(N)(=O)=O)cc1Cl
Mol. weight [g/mol]: 205.66
CAS: 51896-27-6

Physical Properties

Property code	Value	Unit	Source
gf	-312.81	kJ/mol	Joback Method
hf	-409.52	kJ/mol	Joback Method
hfus	27.92	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.296		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	553.94	K	Joback Method
tc	779.33	K	Joback Method
tf	371.85	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.72	J/mol×K	553.94	Joback Method
cpg	295.57	J/mol×K	591.50	Joback Method
cpg	305.72	J/mol×K	629.07	Joback Method
cpg	315.19	J/mol×K	666.63	Joback Method
cpg	323.98	J/mol×K	704.20	Joback Method
cpg	332.07	J/mol×K	741.76	Joback Method
cpg	339.49	J/mol×K	779.33	Joback Method

Sources

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=C51896276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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