P-toluenesulfonamide, n,n-dichloro-

Other names: N,N-dichloro-4-methylbenzenesulfonamide
N,N-dichlorotoluene-4-sulphonamide
Inchi: InChI=1S/C7H7Cl2NO2S/c1-6-2-4-7(5-3-6)13(11,12)10(8)9/h2-5H,1H3
InchiKey: ARGDYOIRHYLIMT-UHFFFAOYSA-N
Formula: C7H7Cl2NO2S
SMILES: Cc1ccc(S(=O)(=O)N(Cl)Cl)cc1
Mol. weight [g/mol]: 240.11
CAS: 473-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-270.78	kJ/mol	Joback Method
hf	-380.05	kJ/mol	Joback Method
hfus	30.33	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-3.51		Aqueous Solubility Prediction Method
logp	2.293		Crippen Method
mcvol	148.280	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	526.30	K	Joback Method
tc	742.49	K	Joback Method
tf	338.46	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.64	J/mol×K	526.30	Joback Method
cpg	301.95	J/mol×K	562.33	Joback Method
cpg	312.49	J/mol×K	598.36	Joback Method
cpg	322.27	J/mol×K	634.40	Joback Method
cpg	331.30	J/mol×K	670.43	Joback Method
cpg	339.62	J/mol×K	706.46	Joback Method

cpg	347.22	J/mol×K	742.49	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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