Benzenesulfonyl chloride, 4-methyl-

Other names:	p-Toluenesulfonyl chloride
	p-Methylbenzenesulfonyl chloride
	p-Toluenesulfochloride
	p-Toluenesulfonic acid chloride
	p-Tolylsulfonyl chloride
	p-Tosyl chloride
	Toluenesulfonyl chloride
	Tosyl chloride
	4-Methylbenzenesulfonyl chloride
	4-Toluenesulfonyl chloride
	Toluene-4-sulfonyl chloride
	Toluene p-sulfonyl chloride
	p-Toluenesulphonyl chloride
	p-Methylphenylsulfonyl chloride
	4-Tosyl chloride
	p-Toluenesulfonic chloride
	4-Toluensulfonyl chloride
	NSC 175822
Inchi:	InChI=1S/C7H7ClO2S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3
InchiKey:	YYROPELSRYBVMQ-UHFFFAOYSA-N
Formula:	C7H7ClO2S
SMILES:	Cc1ccc(S(=O)(=O)Cl)cc1
Mol. weight [g/mol]:	190.65
CAS:	98-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-369.63	kJ/mol	Joback Method
hf	-431.84	kJ/mol	Joback Method
hfus	23.11	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.923		Crippen Method
mcvol	126.060	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	476.43	K	Joback Method
tc	690.41	K	Joback Method

tf	276.07	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.36	J/mol×K	476.43	Joback Method
cpg	245.47	J/mol×K	512.09	Joback Method
cpg	255.96	J/mol×K	547.76	Joback Method
cpg	265.81	J/mol×K	583.42	Joback Method
cpg	275.05	J/mol×K	619.08	Joback Method
cpg	283.68	J/mol×K	654.74	Joback Method
cpg	291.69	J/mol×K	690.41	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=C98599&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