Ethanol, 2-chloro-, 4-methylbenzenesulfonate

Other names:	Ethanol, 2-chloro-, p-toluenesulfonate
	«beta»-Chloroethyl p-toluenesulfonate
	p-Toluenesulfonic acid, 2-chloroethyl ester
	2-(p-Toluenesulfonyloxy)ethyl chloride
	2-Chloroethanol p-toluenesulfonate
	2-Chloroethyl p-toluenesulfonate
	2-Chloroethyl p-tosylate
	2-Chloroethyl tosylate
	2-Chloroethyl para-toluenesulfonate
	«beta»-Chloroethylester kyseliny p-toluensulfonove
	p-Toluenesulfonic acid, «beta»-chloroethyl ester
	2-Chlorethylester kyseliny p-toluensulfonove
	2-Tosyloxyethyl chloride
	Ethanol, 2-chloro-, 1-(4-methylbenzenesulfonate)
	NSC 6079
	2-chloroethyl toluene-4-sulphonate
Inchi:	InChI=1S/C9H11ClO3S/c1-8-2-4-9(5-3-8)14(11,12)13-7-6-10/h2-5H,6-7H2,1H3
InchiKey:	ZXNMIUJDTOMBPV-UHFFFAOYSA-N
Formula:	C9H11ClO3S
SMILES:	Cc1ccc(S(=O)(=O)OCCCl)cc1
Mol. weight [g/mol]:	234.70
CAS:	80-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-457.79	kJ/mol	Joback Method
hf	-605.34	kJ/mol	Joback Method
hfus	29.48	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.939		Crippen Method
mcvol	160.110	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	544.61	K	Joback Method
tc	750.19	K	Joback Method
tf	320.84	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.44	J/mol×K	544.61	Joback Method
cpg	356.40	J/mol×K	578.87	Joback Method
cpg	368.66	J/mol×K	613.14	Joback Method
cpg	380.23	J/mol×K	647.40	Joback Method
cpg	391.10	J/mol×K	681.66	Joback Method
cpg	401.27	J/mol×K	715.93	Joback Method
cpg	410.73	J/mol×K	750.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80411&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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