Benzenesulfonic acid, 4-chlorophenyl ester

Other names:	Benzenesulfonic acid, p-chlorophenyl ester
	p-Chlorophenyl benzenesulfonate
	p-Chlorophenyl benzenesulphonate
	Aracid
	CPBS
	Fenson
	Fensone
	Murvesco
	PCBS
	PCI
	PCPBS
	4-Chlorophenyl benzenesulfonate
	4-Chlorophenyl benzenesulphonate
	928
	(4-Chloor-fenyl)-benzeen-sulfonaat
	(4-Chlor-phenyl)-benzolsulfonat
	(4-Cloro-fenil)-benzol-solfonato
	p-Chlorofenylester kyseliny benzensulfonove
	Ent 4,585
	Fenizon
	GC-928
	Benzenesulfonate de 4-chlorophenyle
	NSC 406662
	Ovicide Seppic
	Phenizon
Inchi:	InChI=1S/C12H9ClO3S/c13-10-6-8-11(9-7-10)16-17(14,15)12-4-2-1-3-5-12/h1-9H
InchiKey:	SPJOZZSIXXJYBT-UHFFFAOYSA-N
Formula:	C12H9ClO2S
SMILES:	O=S(=O)(Oc1ccc(Cl)cc1)c1ccccc1
Mol. weight [g/mol]:	252.72
CAS:	80-38-6

Physical Properties

Property code	Value	Unit	Source
gf	-320.12	kJ/mol	Joback Method
hf	-430.73	kJ/mol	Joback Method

hfus	31.29	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.108		Crippen Method
mcvol	178.620	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	639.93	K	Joback Method
tc	879.02	K	Joback Method
tf	332.42 ± 0.20	K	NIST Webbook
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.44	J/mol×K	639.93	Joback Method
cpg	423.37	J/mol×K	679.78	Joback Method
cpg	436.13	J/mol×K	719.63	Joback Method
cpg	447.73	J/mol×K	759.48	Joback Method
cpg	458.20	J/mol×K	799.32	Joback Method
cpg	467.55	J/mol×K	839.17	Joback Method
cpg	475.80	J/mol×K	879.02	Joback Method
hfust	21.44	kJ/mol	332.20	NIST Webbook
hfust	21.44	kJ/mol	332.20	NIST Webbook

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=C80386&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
hfust:	Enthalpy of fusion at a given temperature
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