Benzene, 1-chloro-4-[(chloromethyl)thio]-

Other names:	Sulfide, chloromethyl p-chlorophenyl (p-Chlorophenylthio)methyl chloride (4-Chlorophenyl)thiomethyl chloride p-Chloro-S-chloromethylbenzenethiol Chloromethyl p-chlorophenyl sulfide Chloromethyl 4-chlorophenyl sulfide Thiophenol, p-chloro-S-chloromethyl p-Chlorfenyl-chlormethylsulfid p-Chlorfenylmerkaptomethylchlorid 1-Chloro-4-(chloromethylthio)benzene p-Chlorophenyl chloromethyl sulfide chloromethyl 4-chlorophenyl sulphide
Inchi:	InChI=1S/C7H6Cl2S/c8-5-10-7-3-1-6(9)2-4-7/h1-4H,5H2
InchiKey:	XPJUCMIJGVAEGF-UHFFFAOYSA-N
Formula:	C7H6Cl2S
SMILES:	ClCSc1ccc(Cl)cc1
Mol. weight [g/mol]:	193.09
CAS:	7205-90-5

Physical Properties

Property code	Value	Unit	Source
gf	120.10	kJ/mol	Joback Method
hf	47.64	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.628		Crippen Method
mcvol	126.560	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	534.86	K	Joback Method
tc	786.07	K	Joback Method
tf	301.83	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.87	J/mol×K	534.86	Joback Method
cpg	237.89	J/mol×K	576.73	Joback Method
cpg	247.16	J/mol×K	618.60	Joback Method
cpg	255.71	J/mol×K	660.46	Joback Method
cpg	263.58	J/mol×K	702.33	Joback Method
cpg	270.78	J/mol×K	744.20	Joback Method
cpg	277.34	J/mol×K	786.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.70	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7205905&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume