3-Chlorothioanisole

Other names: Benzene, 1-chloro-3-(methylthio)-
Inchi: InChI=1S/C7H7ClS/c1-9-7-4-2-3-6(8)5-7/h2-5H,1H3
InchiKey: PTGSDZVASWKUHK-UHFFFAOYSA-N
Formula: C7H7ClS
SMILES: CSc1cccc(Cl)c1
Mol. weight [g/mol]: 158.65
CAS: 4867-37-2

Physical Properties

Property code	Value	Unit	Source
gf	132.03	kJ/mol	Joback Method
hf	63.38	kJ/mol	Joback Method
hfus	15.87	kJ/mol	Joback Method
hvap	45.32	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	3.062		Crippen Method
mcvol	114.320	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	497.43	K	Joback Method
tc	743.67	K	Joback Method
tf	271.91	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.94	J/mol×K	497.43	Joback Method
cpg	216.73	J/mol×K	538.47	Joback Method
cpg	226.81	J/mol×K	579.51	Joback Method
cpg	236.18	J/mol×K	620.55	Joback Method
cpg	244.88	J/mol×K	661.59	Joback Method
cpg	252.92	J/mol×K	702.63	Joback Method
cpg	260.34	J/mol×K	743.67	Joback Method

Sources

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=C4867372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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