Pentachlorothioanisole

Other names:	Benzene, pentachloro(methylthio)-
	Methyl pentachlorophenyl sulfide
	Methylthiopentachlorobenzene
	Pentachloro(methylthio)benzene
	Pentachlorophenyl methyl sulfide
	Sulfide, methyl pentachlorophenyl
	Pctas
	1,2,3,4,5-Pentachloro-6-(methylsulfanyl)benzene
Inchi:	InChI=1S/C7H3Cl5S/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h1H3
InchiKey:	LGZZJTIUEJNNKV-UHFFFAOYSA-N
Formula:	C7H3Cl5S
SMILES:	CSc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	296.43
CAS:	1825-19-0

Physical Properties

Property code	Value	Unit	Source
gf	45.79	kJ/mol	Joback Method
hf	-45.46	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.675		Crippen Method
mcvol	163.280	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	667.07	K	Joback Method
tc	932.24	K	Joback Method
tf	441.67	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.27	J/mol×K	667.07	Joback Method

cpg	284.86	J/mol×K	711.27	Joback Method
cpg	290.91	J/mol×K	755.46	Joback Method
cpg	296.44	J/mol×K	799.66	Joback Method
cpg	301.43	J/mol×K	843.85	Joback Method
cpg	305.88	J/mol×K	888.05	Joback Method
cpg	309.78	J/mol×K	932.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1825190&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