Benzenethiol, pentachloro-

Other names:	Pentachlorobenzenethiol
	Pentachlorothiophenol
	RPA 6
	Pentachlorthiofenol
	USAF B-51
	PCTP
	Akrochem Peptizer PTP
	Pentachlorthiophenol
	Benzenethiol, 2,3,4,5,6-pentachloro-
	NSC 5578
Inchi:	InChI=1S/C6HCl5S/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InchiKey:	LLMLGZUZTFMXSA-UHFFFAOYSA-N
Formula:	C6HCl5S
SMILES:	Sc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	282.40
CAS:	133-49-3

Physical Properties

Property code	Value	Unit	Source
gf	33.64	kJ/mol	Joback Method
hf	-28.21	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.242		Crippen Method
mcvol	149.190	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	638.27	K	Joback Method
tc	911.22	K	Joback Method
tf	432.46	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.45	J/mol×K	638.27	Joback Method
cpg	237.53	J/mol×K	683.76	Joback Method
cpg	242.19	J/mol×K	729.25	Joback Method
cpg	246.46	J/mol×K	774.74	Joback Method
cpg	250.32	J/mol×K	820.24	Joback Method
cpg	253.80	J/mol×K	865.73	Joback Method
cpg	256.90	J/mol×K	911.22	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=C133493&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