4-Chlorobenzyl mercaptan

Other names:	p-Chlorobenzyl mercaptan
	Benzenemethanethiol, 4-chloro-
	p-chlorotoluene-«alpha»-thiol
Inchi:	InChI=1S/C7H7ClS/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2
InchiKey:	GKQXPTHQTXCXEV-UHFFFAOYSA-N
Formula:	C7H7ClS
SMILES:	SCc1ccc(Cl)cc1
Mol. weight [g/mol]:	158.65
CAS:	6258-66-8

Physical Properties

Property code	Value	Unit	Source
gf	128.30	kJ/mol	Joback Method
hf	59.99	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.770		Crippen Method
mcvol	114.320	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	491.51	K	Joback Method
tc	738.23	K	Joback Method
tf	273.97	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.60	J/mol×K	491.51	Joback Method
cpg	215.31	J/mol×K	532.63	Joback Method
cpg	225.26	J/mol×K	573.75	Joback Method
cpg	234.49	J/mol×K	614.87	Joback Method
cpg	243.03	J/mol×K	655.99	Joback Method
cpg	250.92	J/mol×K	697.11	Joback Method

cpg	258.20	J/mol×K	738.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6258668&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