4-Chloro-2-methylthiophenol

Inchi: InChI=1S/C7H7ClS/c1-5-4-6(8)2-3-7(5)9/h2-4,9H,1H3
InchiKey: YIUPEFSJLWXHJR-UHFFFAOYSA-N
Formula: C7H7ClS
SMILES: Cc1cc(Cl)ccc1S
Mol. weight [g/mol]: 158.65
CAS: 17178-01-7

Physical Properties

Property code	Value	Unit	Source
gf	118.67	kJ/mol	Joback Method
hf	48.52	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	45.90	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.937		Crippen Method
mcvol	114.320	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	496.49	K	Joback Method
tc	744.58	K	Joback Method
tf	286.49	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.18	J/mol×K	496.49	Joback Method
cpg	214.44	J/mol×K	537.84	Joback Method
cpg	224.02	J/mol×K	579.19	Joback Method
cpg	232.96	J/mol×K	620.54	Joback Method
cpg	241.28	J/mol×K	661.88	Joback Method
cpg	249.01	J/mol×K	703.23	Joback Method
cpg	256.17	J/mol×K	744.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17178017&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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