4-(Methylthio)thiophenol

Other names: 4-(Methylthio)-benzenethiol
Inchi: InChI=1S/C7H8S2/c1-9-7-4-2-6(8)3-5-7/h2-5,8H,1H3
InchiKey: KYMOWQQIZINTJZ-UHFFFAOYSA-N
Formula: C7H8S2
SMILES: CSc1ccc(S)cc1
Mol. weight [g/mol]: 156.27
CAS: 1122-97-0

Physical Properties

Property code	Value	Unit	Source
gf	173.35	kJ/mol	Joback Method
hf	117.60	kJ/mol	Joback Method
hfus	15.71	kJ/mol	Joback Method
hvap	47.67	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.697		Crippen Method
mcvol	118.430	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
rinpol	1363.00		NIST Webbook
rinpol	1367.00		NIST Webbook
tb	522.86	K	Joback Method
tc	788.46	K	Joback Method
tf	278.45	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.40	J/mol×K	522.86	Joback Method
cpg	236.20	J/mol×K	567.13	Joback Method
cpg	247.16	J/mol×K	611.39	Joback Method
cpg	257.29	J/mol×K	655.66	Joback Method
cpg	266.62	J/mol×K	699.93	Joback Method
cpg	275.17	J/mol×K	744.19	Joback Method

cpg	282.99	J/mol×K	788.46	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=C1122970&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume