Thiazole, 4,5-dihydro-2-(methylthio)-

Other names:	2-(Methylthio)thiazoline
	2-Methylthio-2-thiazoline
	2-Thiazoline, 2-(methylthio)-
	2-(Methylmercapto)-2-thiazoline
	4,5-dihydro-2-(methylthio)thiazole
Inchi:	InChI=1S/C4H7NS2/c1-6-4-5-2-3-7-4/h2-3H2,1H3
InchiKey:	QFGRBBWYHIYNIB-UHFFFAOYSA-N
Formula:	C4H7NS2
SMILES:	CSC1=NCCS1
Mol. weight [g/mol]:	133.24
CAS:	19975-56-5

Physical Properties

Property code	Value	Unit	Source
gf	237.15	kJ/mol	Joback Method
hf	159.34	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.452		Crippen Method
mcvol	94.740	ml/mol	McGowan Method
pc	5438.52	kPa	Joback Method
tb	489.70	K	NIST Webbook
tc	749.85	K	Joback Method
tf	352.65	K	Joback Method
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.05	J/mol×K	485.32	Joback Method
cpg	195.89	J/mol×K	529.41	Joback Method
cpg	206.97	J/mol×K	573.50	Joback Method
cpg	217.30	J/mol×K	617.58	Joback Method

cpg	226.88	J/mol×K	661.67	Joback Method
cpg	235.71	J/mol×K	705.76	Joback Method
cpg	243.79	J/mol×K	749.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19975565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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