Thioacetic acid

Other names:	Methanecarbothiolic acid
	Thioacetic S-acid
	Ethanethioic acid
	Acetyl mercaptan
	Ethanethiolic acid
	Thiacetic acid
	Thiolacetic acid
	Thionoacetic acid
	CH3COSH
	Kyselina thiooctova
	UN 2436
	USAF EK-P-737
	Acetic acid, thio-
Inchi:	InChI=1S/C2H4OS/c1-2(3)4/h1H3,(H,3,4)
InchiKey:	DUYAAUVXQSMXQP-UHFFFAOYSA-N
Formula:	C2H4OS
SMILES:	CC(=O)S
Mol. weight [g/mol]:	76.12
CAS:	507-09-5

Physical Properties

Property code	Value	Unit	Source
chl	-1741.50	kJ/mol	NIST Webbook
gf	-133.57	kJ/mol	Joback Method
hf	-158.71	kJ/mol	Joback Method
hfl	-216.50 ± 0.59	kJ/mol	NIST Webbook
hfl	-219.30 ± 1.50	kJ/mol	NIST Webbook
hfus	6.58	kJ/mol	Joback Method
hvap	33.53	kJ/mol	Joback Method
ie	10.06	eV	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.463		Crippen Method
mcvol	56.960	ml/mol	McGowan Method
pc	6075.01	kPa	Joback Method
ripol	1124.00		NIST Webbook
ripol	1124.00		NIST Webbook
tb	361.89	K	Joback Method

tc	570.61	K	Joback Method
tf	198.69	K	Joback Method
vc	0.207	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.74	J/mol×K	535.82	Joback Method
cpg	82.03	J/mol×K	361.89	Joback Method
cpg	86.54	J/mol×K	396.68	Joback Method
cpg	90.87	J/mol×K	431.46	Joback Method
cpg	95.01	J/mol×K	466.25	Joback Method
cpg	98.96	J/mol×K	501.03	Joback Method
cpg	106.34	J/mol×K	570.61	Joback Method
hvapt	35.20	kJ/mol	333.50	NIST Webbook

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=C507095&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume