Methyl thiolacetate

Other names:	Ethanethioic acid, S-methyl ester
	Acetic acid, thio-, S-methyl ester
	S-Methyl thioacetate
	CH3C(O)SCH3
	Methylthioacetate
	Ethanethioic acid, methyl ester
	Methyl ethanethioate
	S-methyl ethanethioate
Inchi:	InChI=1S/C3H6OS/c1-3(4)5-2/h1-2H3
InchiKey:	OATSQCXMYKYFQO-UHFFFAOYSA-N
Formula:	C3H6OS
SMILES:	CSC(C)=O
Mol. weight [g/mol]:	90.14
CAS:	1534-08-3

Physical Properties

Property code	Value	Unit	Source
affp	829.00	kJ/mol	NIST Webbook
basg	798.00	kJ/mol	NIST Webbook
gf	-121.42	kJ/mol	Joback Method
hf	-175.96	kJ/mol	Joback Method
hfus	9.25	kJ/mol	Joback Method
hvap	35.84	kJ/mol	Joback Method
ie	9.65	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	0.896		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
rinpol	671.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	689.00		NIST Webbook

rinpol	701.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	699.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1054.00		NIST Webbook
ripol	1057.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1041.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1056.00		NIST Webbook
tb	371.30 ± 2.00	K	NIST Webbook
tc	598.06	K	Joback Method
tf	207.90	K	Joback Method
vc	0.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.82	J/mol×K	390.69	Joback Method
cpg	120.17	J/mol×K	425.25	Joback Method
cpg	126.28	J/mol×K	459.81	Joback Method
cpg	132.16	J/mol×K	494.37	Joback Method
cpg	137.80	J/mol×K	528.93	Joback Method
cpg	143.21	J/mol×K	563.49	Joback Method
cpg	148.37	J/mol×K	598.06	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=C1534083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume