Acetic acid, mercapto-, methyl ester

Other names:	Methyl thioglycolate
	Methyl mercaptoacetate
	Methyl 2-mercaptoacetate
	Thioglycolic acid methyl ester
	Methanethiol, methoxy-
	USAF EK-7119
	Thioglykolsaeure-methylester
	Mercaptoacetic acid methyl ester
	Methyl «alpha»-mercaptoacetate
	Methyl ester of thioglycolic acid
	Acetic acid, 2-mercapto-, methyl ester
	NSC 75117
Inchi:	InChI=1S/C3H6O2S/c1-5-3(4)2-6/h6H,2H2,1H3
InchiKey:	MKIJJIMOAABWGF-UHFFFAOYSA-N
Formula:	C3H6O2S
SMILES:	COC(=O)CS
Mol. weight [g/mol]:	106.14
CAS:	2365-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-230.15	kJ/mol	Joback Method
hf	-311.57	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	38.17	kJ/mol	Joback Method
log10ws	-0.01		Crippen Method
logp	0.089		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	5131.32	kPa	Joback Method
rinpol	802.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	791.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1346.00		NIST Webbook
tb	407.19	K	Joback Method
tc	613.74	K	Joback Method

tf	232.19	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.90	J/mol×K	407.19	Joback Method
cpg	138.07	J/mol×K	441.62	Joback Method
cpg	144.07	J/mol×K	476.04	Joback Method
cpg	149.87	J/mol×K	510.47	Joback Method
cpg	155.48	J/mol×K	544.89	Joback Method
cpg	160.88	J/mol×K	579.32	Joback Method
cpg	166.06	J/mol×K	613.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.70	K	1.30	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2365482&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume