2-Methylthioacetic acid

Other names: Acetic acid, (methylthio)-
(methylthio)acetic acid
Inchi: InChI=1S/C3H6O2S/c1-6-2-3(4)5/h2H2,1H3,(H,4,5)
InchiKey: HGTBAIVLETUVCG-UHFFFAOYSA-N
Formula: C3H6O2S
SMILES: CSCC(=O)O
Mol. weight [g/mol]: 106.14
CAS: 2444-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-258.24	kJ/mol	Joback Method
hf	-328.19	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.434		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
tb	482.87	K	Joback Method
tc	679.28	K	Joback Method
tf	268.72	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.94	J/mol×K	482.87	Joback Method
cpg	151.73	J/mol×K	515.60	Joback Method
cpg	157.27	J/mol×K	548.34	Joback Method
cpg	162.56	J/mol×K	581.07	Joback Method
cpg	167.61	J/mol×K	613.81	Joback Method
cpg	172.41	J/mol×K	646.54	Joback Method
cpg	176.96	J/mol×K	679.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	3.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2444373&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume