Acetic acid, mercapto-

Other names:	.alpha.-mercaptoacetic acid
	2-mercaptoacetic acid
	2-mercaptoethanoic acid
	2-thioglycolic acid
	Acetic acid, 2-mercapto-
	Acide thioglycolique
	Glycolic acid, thio-
	Kyselina merkaptooctova
	Kyselina thioglykolova
	NSC 1894
	Thioglycollic acid
	UN 1940
	USAF CB-35
	glycolic acid, 2-thio-
	mercaptoacetic acid
	thioglycolic acid
	thiovanic acid
	«alpha»-Mercaptoacetic acid
Inchi:	InChI=1S/C2H4O2S/c3-2(4)1-5/h5H,1H2,(H,3,4)
InchiKey:	CWERGRDVMFNCDR-UHFFFAOYSA-N
Formula:	C2H4O2S
SMILES:	O=C(O)CS
Mol. weight [g/mol]:	92.12
CAS:	68-11-1

Physical Properties

Property code	Value	Unit	Source
gf	-270.39	kJ/mol	Joback Method
hf	-310.94	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	50.21	kJ/mol	Joback Method
log10ws	0.17		Crippen Method
logp	8.000e-04		Crippen Method
mcvol	62.830	ml/mol	McGowan Method
pc	7049.79	kPa	Joback Method
tb	454.07	K	Joback Method
tc	652.94	K	Joback Method

tf	259.51	K	Joback Method
vc	0.227	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.68	J/mol×K	586.65	Joback Method
cpg	128.13	J/mol×K	619.80	Joback Method
cpg	108.95	J/mol×K	454.07	Joback Method
cpg	113.18	J/mol×K	487.22	Joback Method
cpg	117.21	J/mol×K	520.36	Joback Method
cpg	121.04	J/mol×K	553.51	Joback Method
cpg	131.40	J/mol×K	652.94	Joback Method
hvapt	56.80	kJ/mol	380.00	NIST Webbook
rfi	1.50270		293.15	Isobaric Vapor Liquid Equilibrium for Binary Systems of Thioglycolic Acid with Water, Butyl Acetate, Butyl Formate, and Isobutyl Acetate at 101.3 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	0.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Liquid-liquid equilibrium measurement and thermodynamics modeling for the systems water + thioglycolic acid + isopropyl ether/methyl tert-butyl ether at 298.15 and 308.15 K: https://www.doi.org/10.1016/j.fluid.2018.08.003

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68111&Units=SI

CrippenMethod: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Liquid-Liquid Equilibria for the Ternary Systems of Water + Thioglycolic Acid + 2-Ethyl-1-hexyl Thioglycolate and Water + 2-Ethyl-1-hexyl Thioglycolate + 2-Ethyl-1-hexanol at 293.15, 303.15, and 313.15 K under Atmospheric Pressure: Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for extraction of thioglycolic acid from aqueous solution with different solvents: Liquid-Liquid Equilibrium for Ternary Systems of Thioglycolic Acid with Water, Butyl Acetate, Butyl Formate, and Isobutyl Acetate at 101.3 kPa: https://www.doi.org/10.1021/acs.jced.8b00619

Separation of thioglycolic acid from its aqueous solution by ionic liquids: Ionic liquid and liquid-liquid phase equilibrium: https://www.doi.org/10.1016/j.jct.2017.12.007

Joback Method: In the COSMO-SAC model: https://en.wikipedia.org/wiki/Joback_method

https://www.doi.org/10.1016/j.jct.2017.06.015

https://www.doi.org/10.1021/acs.jced.6b00686

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rfi:	Refractive Index
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume