3-Mercaptopropionic acid

Other names:	2-Mercaptoethanecarboxylic acid
	3-Mercaptopropanoic acid
	3-Thiolpropanoic acid
	3-Thiopropanoic acid
	3-Thiopropionic acid
	3MPA
	Hydracrylic acid, 3-thio-
	Mercaptopropionic acid
	NSC 437
	Propanoic acid, 3-mercapto-
	Propionic acid, 3-mercapto-
	«beta»-Mercaptopropanoic acid
	«beta»-Mercaptopropionic acid
	«beta»-Thiopropionic acid
	Â«betaÂ»-Mercaptopropanoic acid
	Â«betaÂ»-Mercaptopropionic acid
	Â«betaÂ»-Thiopropionic acid
Inchi:	InChI=1S/C3H6O2S/c4-3(5)1-2-6/h6H,1-2H2,(H,4,5)
InchiKey:	DKIDEFUBRARXTE-UHFFFAOYSA-N
Formula:	C3H6O2S
SMILES:	O=C(O)CCS
Mol. weight [g/mol]:	106.14
CAS:	107-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-261.97	kJ/mol	Joback Method
hf	-331.58	kJ/mol	Joback Method
hfus	13.25	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	0.391		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	6037.30	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
ripol	2193.00		NIST Webbook

ripol	2193.00		NIST Webbook
sl	228.90	J/mol×K	NIST Webbook
tb	476.95	K	Joback Method
tc	673.43	K	Joback Method
tf	270.78	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.21	J/mol×K	476.95	Joback Method
cpg	150.89	J/mol×K	509.70	Joback Method
cpg	156.30	J/mol×K	542.44	Joback Method
cpg	161.44	J/mol×K	575.19	Joback Method
cpg	166.33	J/mol×K	607.94	Joback Method
cpg	170.96	J/mol×K	640.69	Joback Method
cpg	175.36	J/mol×K	673.43	Joback Method
cpl	202.50	J/mol×K	299.80	NIST Webbook
hfust	16.97	kJ/mol	291.90	NIST Webbook
hfust	16.97	kJ/mol	291.90	NIST Webbook
sfust	58.20	J/mol×K	291.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	2.00	NIST Webbook
tbrp	358.70	K	0.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibrium for the Ternary System of 3-Mercaptopropionic Acid + Water + Trichloromethane:	https://www.doi.org/10.1021/acs.jced.8b01187

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume