2-Mercaptopropanoic acid

Other names:	Thiolactic acid
	2-Mercaptopropionic acid
	Propanoic acid, 2-mercapto-
	Propionic acid, 2-mercapto-
	«alpha»-Mercaptopropanoic acid
	«alpha»-Mercaptopropionic acid
	2-Thiolactic acid
	UN 2936
	2-Sulfanylpropanoic acid
Inchi:	InChI=1S/C3H6O2S/c1-2(6)3(4)5/h2,6H,1H3,(H,4,5)
InchiKey:	PMNLUUOXGOOLSP-UHFFFAOYSA-N
Formula:	C3H6O2S
SMILES:	CC(S)C(=O)O
Mol. weight [g/mol]:	106.14
CAS:	79-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-264.41	kJ/mol	Joback Method
hf	-336.86	kJ/mol	Joback Method
hfus	9.73	kJ/mol	Joback Method
hvap	52.05	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	0.389		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	6113.06	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2130.00		NIST Webbook
tb	476.51	K	Joback Method
tc	677.47	K	Joback Method
tf	255.78	K	Joback Method
tt	291.90 ± 0.20	K	NIST Webbook
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.49	J/mol×K	476.51	Joback Method
cpg	151.38	J/mol×K	510.00	Joback Method
cpg	156.98	J/mol×K	543.50	Joback Method
cpg	162.29	J/mol×K	576.99	Joback Method
cpg	167.32	J/mol×K	610.48	Joback Method
cpg	172.09	J/mol×K	643.97	Joback Method
cpg	176.58	J/mol×K	677.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.20	K	2.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79425&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
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
tt:	Triple Point Temperature
vc:	Critical Volume