Propanoic acid, 3-mercapto-, methyl ester

Other names:	Propionic acid, 3-mercapto-, methyl ester
	Methyl «beta»-mercaptopropionate
	Methyl 3-mercaptopropionate
	3-Mercaptopropionic acid methyl ester
	Methyl mercaptopropionate
Inchi:	InChI=1S/C4H8O2S/c1-6-4(5)2-3-7/h7H,2-3H2,1H3
InchiKey:	LDTLDBDUBGAEDT-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	COC(=O)CCS
Mol. weight [g/mol]:	120.17
CAS:	2935-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-221.73	kJ/mol	Joback Method
hf	-332.21	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.479		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	430.07	K	Joback Method
tc	634.41	K	Joback Method
tf	243.46	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.85	J/mol×K	430.07	Joback Method
cpg	174.67	J/mol×K	464.13	Joback Method
cpg	182.21	J/mol×K	498.18	Joback Method
cpg	189.48	J/mol×K	532.24	Joback Method

cpg	196.47	J/mol×K	566.30	Joback Method
cpg	203.17	J/mol×K	600.36	Joback Method
cpg	209.57	J/mol×K	634.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.70	K	1.90	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=C2935902&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume