Propanoic acid, 2-mercapto-, methyl ester

Other names:	Methyl 2-mercaptopropionate
	Methyl «alpha»-mercaptopropionate
	«alpha»-Mercaptopropionic acid methyl ester
	Methyl alpha-mercaptopropionate
Inchi:	InChI=1S/C4H8O2S/c1-3(7)4(5)6-2/h3,7H,1-2H3
InchiKey:	SNWKNPMDQONHKK-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	COC(=O)C(C)S
Mol. weight [g/mol]:	120.17
CAS:	53907-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-224.17	kJ/mol	Joback Method
hf	-337.49	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	40.00	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	0.478		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	813.00		NIST Webbook
tb	429.63	K	Joback Method
tc	638.94	K	Joback Method
tf	228.46	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.98	J/mol×K	429.63	Joback Method
cpg	175.08	J/mol×K	464.52	Joback Method
cpg	182.89	J/mol×K	499.40	Joback Method
cpg	190.40	J/mol×K	534.29	Joback Method

cpg	197.60	J/mol×K	569.17	Joback Method
cpg	204.49	J/mol×K	604.06	Joback Method
cpg	211.07	J/mol×K	638.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53907463&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume