N-3-(Methylthio)propyl O-methyl thiocarbamate

Inchi: InChI=1S/C6H13NOS2/c1-8-6(9)7-4-3-5-10-2/h3-5H2,1-2H3,(H,7,9)
InchiKey: GWPFPKJDKKYAPM-UHFFFAOYSA-N
Formula: C6H13NOS2
SMILES: COC(S)=NCCCSC
Mol. weight [g/mol]: 179.30

Physical Properties

Property code	Value	Unit	Source
hf	-146.61	kJ/mol	Joback Method
hvap	48.31	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.672		Crippen Method
mcvol	139.650	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	567.30	K	Joback Method
tc	800.33	K	Joback Method

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=R440003&Units=SI

Legend

hf: Enthalpy of formation 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
tc:	Critical Temperature