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

Inchi: InChI=1S/C7H15NOS2/c1-3-9-7(10)8-5-4-6-11-2/h3-6H2,1-2H3,(H,8,10)
InchiKey: ILEAFLQTFMPPOU-UHFFFAOYSA-N
Formula: C7H15NOS2
SMILES: CCOC(=S)NCCCSC
Mol. weight [g/mol]: 193.33
CAS: 89855-25-4

Physical Properties

Property code	Value	Unit	Source
gf	142.63	kJ/mol	Joback Method
hf	-78.19	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.651		Crippen Method
mcvol	153.740	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1620.00		NIST Webbook
ripol	2696.00		NIST Webbook
tb	570.97	K	Joback Method
tc	783.59	K	Joback Method
tf	312.21	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/mol×K	570.97	Joback Method
cpg	360.52	J/mol×K	606.41	Joback Method
cpg	372.11	J/mol×K	641.84	Joback Method
cpg	383.04	J/mol×K	677.28	Joback Method
cpg	393.34	J/mol×K	712.72	Joback Method
cpg	403.05	J/mol×K	748.16	Joback Method
cpg	412.19	J/mol×K	783.59	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=C89855254&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume