Ethanethioic acid, (methylthio)-s-ethyl ester

Inchi: InChI=1S/C5H10OS2/c1-3-8-5(6)4-7-2/h3-4H2,1-2H3
InchiKey: SQROSXWNNSGURE-UHFFFAOYSA-N
Formula: C5H10OS2
SMILES: CCSC(=O)CSC
Mol. weight [g/mol]: 150.26
CAS: 119152-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-71.46	kJ/mol	Joback Method
hf	-175.37	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
ie	8.62	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.629		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	505.23	K	Joback Method
tc	731.16	K	Joback Method
tf	264.84	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.90	J/mol×K	505.23	Joback Method
cpg	237.07	J/mol×K	542.89	Joback Method
cpg	246.75	J/mol×K	580.54	Joback Method
cpg	255.93	J/mol×K	618.20	Joback Method
cpg	264.60	J/mol×K	655.85	Joback Method
cpg	272.76	J/mol×K	693.51	Joback Method
cpg	280.40	J/mol×K	731.16	Joback Method

Sources

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=C119152817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume