Ethyl thioformate

Inchi: InChI=1S/C3H6OS/c1-2-5-3-4/h3H,2H2,1H3
InchiKey: STSBSFZTOFGGKP-UHFFFAOYSA-N
Formula: C3H6OS
SMILES: CCSC=O
Mol. weight [g/mol]: 90.14
CAS: 21071-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-92.02	kJ/mol	Joback Method
hf	-177.70 ± 5.10	kJ/mol	NIST Webbook
hfl	-216.00 ± 2.60	kJ/mol	NIST Webbook
hfus	9.94	kJ/mol	Joback Method
hvap	38.20 ± 4.20	kJ/mol	NIST Webbook
log10ws	-5.38		Crippen Method
logp	0.930		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	385.48	K	Joback Method
tc	586.69	K	Joback Method
tf	199.97	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.50	J/mol×K	385.48	Joback Method
cpg	122.57	J/mol×K	419.01	Joback Method
cpg	128.42	J/mol×K	452.55	Joback Method
cpg	134.05	J/mol×K	486.08	Joback Method
cpg	139.45	J/mol×K	519.62	Joback Method
cpg	144.62	J/mol×K	553.15	Joback Method
cpg	149.57	J/mol×K	586.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21071396&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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume