Thioacetic acid, O-ethyl ester

Other names:	CH3C(S)OCH2CH3
	Ethyl thionacetate
Inchi:	InChI=1S/C4H8OS/c1-3-5-4(2)6/h3H2,1-2H3
InchiKey:	IEPFHYMMMGMRNF-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CCOC(C)=S
Mol. weight [g/mol]:	104.17
CAS:	926-67-0

Physical Properties

Property code	Value	Unit	Source
affp	863.60	kJ/mol	NIST Webbook
basg	831.80	kJ/mol	NIST Webbook
gf	-5.14	kJ/mol	Joback Method
hf	-111.61	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	33.64	kJ/mol	Joback Method
ie	8.82	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.370		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	383.38	K	Joback Method
tc	580.19	K	Joback Method
tf	191.34	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.98	J/mol×K	383.38	Joback Method
cpg	150.69	J/mol×K	416.18	Joback Method
cpg	158.01	J/mol×K	448.98	Joback Method
cpg	164.94	J/mol×K	481.79	Joback Method

cpg	171.52	J/mol×K	514.59	Joback Method
cpg	177.76	J/mol×K	547.39	Joback Method
cpg	183.67	J/mol×K	580.19	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=C926670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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