S-Ethyl ethanethioate

Other names:	Acetic acid, thio-, S-ethyl ester
	Ethyl thiolacetate
	S-Ethyl thioacetate
	S-Ethyl thiolacetate
	Ethanethioic acid, S-ethyl ester
	CH3COSC2H5
	Ethyl thioacetate
Inchi:	InChI=1S/C4H8OS/c1-3-6-4(2)5/h3H2,1-2H3
InchiKey:	APTGPWJUOYMUCE-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CCSC(C)=O
Mol. weight [g/mol]:	104.17
CAS:	625-60-5

Physical Properties

Property code	Value	Unit	Source
gf	-113.00	kJ/mol	Joback Method
hf	-227.80 ± 0.92	kJ/mol	NIST Webbook
hfl	-267.80 ± 0.88	kJ/mol	NIST Webbook
hfus	11.84	kJ/mol	Joback Method
hvap	40.00 ± 0.20	kJ/mol	NIST Webbook
hvap	40.00 ± 0.20	kJ/mol	NIST Webbook
hvap	40.00 ± 0.20	kJ/mol	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	1.286		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4075.00 ± 80.00	kPa	NIST Webbook
rhoc	327.10 ± 10.00	kg/m3	NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	749.00		NIST Webbook
ripol	1080.00		NIST Webbook

ripol	1092.00		NIST Webbook
ripol	1109.00		NIST Webbook
tb	389.60	K	NIST Webbook
tb	386.90 ± 2.00	K	NIST Webbook
tc	590.55 ± 0.20	K	NIST Webbook
tf	219.17	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.97	J/mol×K	413.57	Joback Method
cpg	155.97	J/mol×K	447.80	Joback Method
cpg	163.66	J/mol×K	482.03	Joback Method
cpg	171.03	J/mol×K	516.25	Joback Method
cpg	178.09	J/mol×K	550.48	Joback Method
cpg	184.83	J/mol×K	584.71	Joback Method
cpg	191.25	J/mol×K	618.94	Joback Method

Sources

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=C625605&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhoc:	Critical density
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