Ethanethioic acid, trifluoro-, S-ethyl ester

Other names:	Acetic acid, trifluorothio-, S-ethyl ester
	Ethanethioic acid, 2,2,2-trifluoro-, S-ethyl ester
	Ethyl trifluorothioacetate
	Ethyl trifluorothiolacetate
	NSC 88936
	S-Ethyl trifluoroethanethioate
	S-Ethyl trifluorothioacetate
	S-Ethylthioltrifluoroacetate
	S-Ethylthiotrifluoroacetate
	Trifluoroethanethioic acid S-ethyl ester
	Trifluorothioacetic acid S-ethyl ester
Inchi:	InChI=1S/C4H5F3OS/c1-2-9-3(8)4(5,6)7/h2H2,1H3
InchiKey:	VGGUKFAVHPGNBF-UHFFFAOYSA-N
Formula:	C4H5F3OS
SMILES:	CCSC(=O)C(F)(F)F
Mol. weight [g/mol]:	158.14
CAS:	383-64-2

Physical Properties

Property code	Value	Unit	Source
gf	-694.59	kJ/mol	Joback Method
hf	-815.50 ± 7.90	kJ/mol	NIST Webbook
hfl	-851.90 ± 4.10	kJ/mol	NIST Webbook
hfus	13.67	kJ/mol	Joback Method
hvap	36.00 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.828		Crippen Method
mcvol	90.450	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	363.70	K	NIST Webbook
tc	593.68	K	Joback Method
tf	223.36	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.47	J/mol×K	408.15	Joback Method
cpg	183.43	J/mol×K	439.07	Joback Method
cpg	190.94	J/mol×K	469.99	Joback Method
cpg	198.00	J/mol×K	500.91	Joback Method
cpg	204.64	J/mol×K	531.84	Joback Method
cpg	210.86	J/mol×K	562.76	Joback Method
cpg	216.70	J/mol×K	593.68	Joback Method
hvapt	42.00	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	8.84322e+00
Coeff. B	-8.51201e+02
Coeff. C	-1.62277e+02
Temperature range (K), min.	261.77
Temperature range (K), max.	403.29

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=C383642&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume