Ethanethioic acid, S-propyl ester

Other names:	Acetic acid, thio-, S-propyl ester
	Propyl thiolacetate
	S-Propyl thioacetate
	Propyl thioacetate
	S-n-Propyl thioacetate
	S-propyl ethanethioate
Inchi:	InChI=1S/C5H10OS/c1-3-4-7-5(2)6/h3-4H2,1-2H3
InchiKey:	SBWFWBJCYMBZEY-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CCCSC(C)=O
Mol. weight [g/mol]:	118.20
CAS:	2307-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-104.58	kJ/mol	Joback Method
hf	-217.24	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	44.10 ± 0.20	kJ/mol	NIST Webbook
hvap	44.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.57		Crippen Method
logp	1.676		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	877.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	851.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1160.00		NIST Webbook
tb	409.20	K	NIST Webbook
tb	411.40 ± 3.00	K	NIST Webbook
tc	639.57	K	Joback Method
tf	230.44	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.53	J/mol×K	436.45	Joback Method
cpg	194.04	J/mol×K	470.30	Joback Method
cpg	203.15	J/mol×K	504.16	Joback Method
cpg	211.86	J/mol×K	538.01	Joback Method
cpg	220.19	J/mol×K	571.86	Joback Method
cpg	228.12	J/mol×K	605.72	Joback Method
cpg	235.68	J/mol×K	639.57	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=C2307100&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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