Ethanethioic acid, S-(1-methylethyl) ester

Other names:	Acetic acid, thio-, S-isopropyl ester
	Isopropyl thiolacetate
	S-Isopropyl thioacetate
	Ethanethioic acid S-(isopropyl) ester
	CH3C(O)SCH(CH3)2
Inchi:	InChI=1S/C5H10OS/c1-4(2)7-5(3)6/h4H,1-3H3
InchiKey:	XBSWGFUCFLITEY-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CC(=O)SC(C)C
Mol. weight [g/mol]:	118.20
CAS:	926-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-107.02	kJ/mol	Joback Method
hf	-222.52	kJ/mol	Joback Method
hfus	10.91	kJ/mol	Joback Method
hvap	42.30 ± 0.20	kJ/mol	NIST Webbook
hvap	42.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.674		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
tb	398.00 ± 2.00	K	NIST Webbook
tc	644.03	K	Joback Method
tf	215.44	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.66	J/mol×K	436.01	Joback Method

cpg	194.48	J/mol×K	470.68	Joback Method
cpg	203.89	J/mol×K	505.35	Joback Method
cpg	212.87	J/mol×K	540.02	Joback Method
cpg	221.43	J/mol×K	574.69	Joback Method
cpg	229.58	J/mol×K	609.36	Joback Method
cpg	237.31	J/mol×K	644.03	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=C926738&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume