Ethyl (methylthio)acetate

Other names:	Ethyl «alpha»(methylthio)acetate
	Methylthioacetic acid ethyl ester
	Acetic acid, (methylthio)-, ethyl ester
	Ethyl 2-(methylthio)acetate
	Methylsulfanyl-acetic acid ethyl ester
Inchi:	InChI=1S/C5H10O2S/c1-3-7-5(6)4-8-2/h3-4H2,1-2H3
InchiKey:	MDIAKIHKBBNYHF-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	CCOC(=O)CSC
Mol. weight [g/mol]:	134.20
CAS:	4455-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-209.58	kJ/mol	Joback Method
hf	-349.46	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	42.70	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
log10ws	-0.66		Crippen Method
logp	0.913		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	979.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	981.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1438.00		NIST Webbook

ripol	1434.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1451.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1450.00		NIST Webbook
tb	458.87	K	Joback Method
tc	660.77	K	Joback Method
tf	252.67	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.45	J/mol×K	458.87	Joback Method
cpg	214.81	J/mol×K	492.52	Joback Method
cpg	223.85	J/mol×K	526.17	Joback Method
cpg	232.56	J/mol×K	559.82	Joback Method
cpg	240.93	J/mol×K	593.47	Joback Method
cpg	248.95	J/mol×K	627.12	Joback Method
cpg	256.60	J/mol×K	660.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.20	K	3.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4455134&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume