3-(Methylthio)propanoic acid methyl ester

Other names:	Propionic acid, 3-(methylthio)-, methyl ester
	Methyl «beta»-methylmercaptopropionate
	Methyl «beta»-methylthiopropionate
	Methyl 3-(methylthio)propionate
	Methyl-3-methylmercaptopropionate
	Propanoic acid, 3-(methylthio)-, methyl ester
	Methyl ester of 3-(methylthio)propanoic acid
	Methyl 3-(methylsulfanyl)propanoate
	Methyl 3-methylthiopropanoate
	NSC 76415
	2-Methoxycarbonylethyl methyl sulfide
Inchi:	InChI=1S/C5H10O2S/c1-7-5(6)3-4-8-2/h3-4H2,1-2H3
InchiKey:	DMMJVMYCBULSIS-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	COC(=O)CCSC
Mol. weight [g/mol]:	134.20
CAS:	13532-18-8

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
log10ws	-0.66		Crippen Method
logp	0.913		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1026.80		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1023.00		NIST Webbook

ripol	1516.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1510.00		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	347.70	K	1.70	NIST Webbook

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=C13532188&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
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