Propanoic acid, 3-(methylthio)-, 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

Physical Properties

Property code	Value	Unit	Source
af	0.4045		Cheméo Relay (1.0)
hf	-405.11	kJ/mol	Cheméo Relay (1.0)
hfus	15.62	kJ/mol	Joback Method
hvap	54.76	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-0.09		Cheméo Relay (1.0)
logp	0.913		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1023.00		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
rinpol	1027.00		NIST Webbook
rinpol	1000.00		NIST Webbook

ripol	1510.00		NIST Webbook
ripol	1516.00		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	1540.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	451.96	K	Cheméo Relay (1.0)
tc	640.20	K	Cheméo Relay (1.0)
tf	224.98	K	Cheméo Relay (1.0)
vc	0.366	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13532188&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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