Methyl 3-(methylthio)-(Z)-2-propenoate

Other names: (Z)-2-Propenoic acid, 3-methylthio-, methyl ester
Methyl 3-(methylthio)-2-propenoate, (Z)
Inchi: InChI=1S/C5H8O2S/c1-7-5(6)3-4-8-2/h3-4H,1-2H3/b4-3-
InchiKey: KAFIOMPFBSDFPP-ARJAWSKDSA-N
Formula: C5H8O2S
SMILES: COC(=O)C=CSC
Mol. weight [g/mol]: 132.18
CAS: 15904-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-129.36	kJ/mol	Joback Method
hf	-232.24	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	42.66	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.036		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1076.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1773.00		NIST Webbook
tb	463.03	K	Joback Method
tc	675.06	K	Joback Method
tf	247.59	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.44	J/mol×K	463.03	Joback Method
cpg	197.25	J/mol×K	498.37	Joback Method
cpg	205.66	J/mol×K	533.71	Joback Method
cpg	213.69	J/mol×K	569.05	Joback Method

cpg	221.33	J/mol×K	604.38	Joback Method
cpg	228.58	J/mol×K	639.72	Joback Method
cpg	235.46	J/mol×K	675.06	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=C15904844&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