Ethyl 3-(methylthio)-(E)-2-propenoate

Other names: (E)-2-Propenoic acid, 3-methylthio-, ethyl ester
Ethyl 3-(methylthio)-2-propenoate, (E)
Inchi: InChI=1S/C6H10O2S/c1-3-8-6(7)4-5-9-2/h4-5H,3H2,1-2H3/b5-4+
InchiKey: DNNJFSSUXIAKAI-SNAWJCMRSA-N
Formula: C6H10O2S
SMILES: CCOC(=O)C=CSC
Mol. weight [g/mol]: 146.21
CAS: 136115-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-120.94	kJ/mol	Joback Method
hf	-252.88	kJ/mol	Joback Method
hfus	18.42	kJ/mol	Joback Method
hvap	44.88	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.426		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1733.00		NIST Webbook
tb	485.91	K	Joback Method
tc	694.93	K	Joback Method
tf	258.86	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.96	J/mol×K	485.91	Joback Method
cpg	238.11	J/mol×K	520.75	Joback Method
cpg	247.80	J/mol×K	555.58	Joback Method
cpg	257.02	J/mol×K	590.42	Joback Method
cpg	265.79	J/mol×K	625.25	Joback Method
cpg	274.11	J/mol×K	660.09	Joback Method
cpg	281.98	J/mol×K	694.93	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=C136115656&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume