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=C/SC
Mol. weight [g/mol]: 146.21

Physical Properties

Property code	Value	Unit	Source
af	0.3929		Cheméo Relay (1.0)
hf	-361.99	kJ/mol	Cheméo Relay (1.0)
hfus	18.42	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.426		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1733.00		NIST Webbook
tb	478.05	K	Cheméo Relay (1.0)
tc	641.60	K	Cheméo Relay (1.0)
tf	258.38	K	Cheméo Relay (1.0)
vc	0.398	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C136115656&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

Cheméo Relay (1.0):

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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume