

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

Other names:	(Z)-2-Propenoic acid, 3-methylthio-, ethyl ester Ethyl 3-(methylthio)-2-propenoate, (Z)
Inchi:	InChI=1S/C6H10O2S/c1-3-8-6(7)4-5-9-2/h4-5H,3H2,1-2H3/b5-4-
InchiKey:	DNNJFSSUXIAKAI-PLNGDYQASA-N
Formula:	C6H10O2S
SMILES:	CCOC(=O)C=CSC
Mol. weight [g/mol]:	146.21
CAS:	136115-66-7

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	1158.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1824.00		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/molxK	485.91	Joback Method
cpg	238.11	J/molxK	520.75	Joback Method
cpg	247.80	J/molxK	555.58	Joback Method
cpg	257.02	J/molxK	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=C136115667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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