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

Inchi: InChI=1S/C7H12O2S/c1-3-5-9-7(8)4-6-10-2/h4,6H,3,5H2,1-2H3/b6-4+
InchiKey: UZTNLELOESZULR-GQCTYLIASA-N
Formula: C7H12O2S
SMILES: CCCOC(=O)C=CSC
Mol. weight [g/mol]: 160.23

Physical Properties

Property code	Value	Unit	Source
gf	-112.52	kJ/mol	Joback Method
hf	-273.52	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	47.11	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.816		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
ripol	1827.00		NIST Webbook
tb	508.79	K	Joback Method
tc	714.76	K	Joback Method
tf	270.13	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.59	J/mol×K	508.79	Joback Method
cpg	280.93	J/mol×K	543.12	Joback Method
cpg	291.74	J/mol×K	577.45	Joback Method
cpg	302.03	J/mol×K	611.78	Joback Method
cpg	311.80	J/mol×K	646.11	Joback Method
cpg	321.06	J/mol×K	680.43	Joback Method
cpg	329.81	J/mol×K	714.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R327361&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume