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

Inchi: InChI=1S/C11H20O2S/c1-3-4-5-6-9-13-11(12)8-7-10-14-2/h7-8H,3-6,9-10H2,1-2H3/b8-7
InchiKey: XGLNTMGQKLCXSS-BQYQJAHWSA-N
Formula: C11H20O2S
SMILES: CCCCCCOC(=O)C=CCSC
Mol. weight [g/mol]: 216.34

Physical Properties

Property code	Value	Unit	Source
gf	-78.84	kJ/mol	Joback Method
hf	-356.08	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	56.01	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.029		Crippen Method
mcvol	185.340	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
ripol	2154.00		NIST Webbook
ripol	2154.00		NIST Webbook
tb	600.31	K	Joback Method
tc	795.00	K	Joback Method
tf	315.21	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.01	J/mol×K	600.31	Joback Method
cpg	469.81	J/mol×K	632.76	Joback Method
cpg	483.88	J/mol×K	665.21	Joback Method
cpg	497.24	J/mol×K	697.66	Joback Method
cpg	509.90	J/mol×K	730.11	Joback Method
cpg	521.88	J/mol×K	762.55	Joback Method
cpg	533.20	J/mol×K	795.00	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=R395661&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