(Z)-3-hexenyl 3-(methylthio)propanoate

Inchi: InChI=1S/C10H18O2S/c1-3-4-5-6-8-12-10(11)7-9-13-2/h4-5H,3,6-9H2,1-2H3/b5-4-
InchiKey: YQYJLDYTWFXZNJ-PLNGDYQASA-N
Formula: C10H18O2S
SMILES: CCC=CCCOC(=O)CCSC
Mol. weight [g/mol]: 202.31

Physical Properties

Property code	Value	Unit	Source
gf	-87.26	kJ/mol	Joback Method
hf	-335.44	kJ/mol	Joback Method
hfus	28.78	kJ/mol	Joback Method
hvap	53.78	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.639		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	577.43	K	Joback Method
tc	774.70	K	Joback Method
tf	303.94	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.03	J/mol×K	577.43	Joback Method
cpg	420.14	J/mol×K	610.31	Joback Method
cpg	433.55	J/mol×K	643.19	Joback Method
cpg	446.30	J/mol×K	676.07	Joback Method
cpg	458.38	J/mol×K	708.95	Joback Method
cpg	469.82	J/mol×K	741.82	Joback Method
cpg	480.63	J/mol×K	774.70	Joback Method

Sources

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=R327425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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