5-methyl-2-[(methylthio)methyl]-2-hexenal

Inchi: InChI=1S/C9H16OS/c1-8(2)4-5-9(6-10)7-11-3/h5-6,8H,4,7H2,1-3H3/b9-5-
InchiKey: FHZUYUPNOHOVIC-UITAMQMPSA-N
Formula: C9H16OS
SMILES: CSCC(C=O)=CCC(C)C
Mol. weight [g/mol]: 172.29

Physical Properties

Property code	Value	Unit	Source
gf	27.73	kJ/mol	Joback Method
hf	-170.65	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.521		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	526.36	K	Joback Method
tc	731.35	K	Joback Method
tf	233.55	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.47	J/mol×K	526.36	Joback Method
cpg	349.25	J/mol×K	560.52	Joback Method
cpg	362.29	J/mol×K	594.69	Joback Method
cpg	374.63	J/mol×K	628.85	Joback Method
cpg	386.29	J/mol×K	663.02	Joback Method
cpg	397.30	J/mol×K	697.18	Joback Method
cpg	407.68	J/mol×K	731.35	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=R308197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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