5-Methyl-4-mercaptohexyl-2-acetate, # 1

Inchi: InChI=1S/C9H18O2S/c1-6(2)9(12)5-7(3)11-8(4)10/h6-7,9,12H,5H2,1-4H3
InchiKey: XCOUODRDDWCWCD-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CC(=O)OC(C)CC(S)C(C)C
Mol. weight [g/mol]: 190.30

Physical Properties

Property code	Value	Unit	Source
gf	-186.95	kJ/mol	Joback Method
hf	-451.25	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.283		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1224.00		NIST Webbook
rinpol	1224.00		NIST Webbook
tb	543.15	K	Joback Method
tc	747.37	K	Joback Method
tf	254.81	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.02	J/mol×K	543.15	Joback Method
cpg	390.80	J/mol×K	577.19	Joback Method
cpg	404.88	J/mol×K	611.22	Joback Method
cpg	418.25	J/mol×K	645.26	Joback Method
cpg	430.94	J/mol×K	679.30	Joback Method
cpg	442.94	J/mol×K	713.34	Joback Method
cpg	454.27	J/mol×K	747.37	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=R603239&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume