5-Methyl-4-mercaptohexyl-2-acetate

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	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1224.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		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

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=R291891&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume