3-(Methylthio)hexyl acetate

Other names: 1-Hexanol, 3-(methylthio)-, 1-acetate
acetato 3-metiltio-1-hexilo
Inchi: InChI=1S/C9H18O2S/c1-4-5-9(12-3)6-7-11-8(2)10/h9H,4-7H2,1-3H3
InchiKey: VIQXICKUKPVFRK-UHFFFAOYSA-N
Formula: C9H18O2S
SMILES: CCCC(CCOC(C)=O)SC
Mol. weight [g/mol]: 190.30
CAS: 51755-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-178.34	kJ/mol	Joback Method
hf	-437.30	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.471		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
ripol	1766.00		NIST Webbook
ripol	1749.00		NIST Webbook
tb	549.95	K	Joback Method
tc	745.63	K	Joback Method
tf	282.75	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.02	J/mol×K	549.95	Joback Method
cpg	392.14	J/mol×K	582.56	Joback Method
cpg	405.64	J/mol×K	615.18	Joback Method
cpg	418.52	J/mol×K	647.79	Joback Method
cpg	430.78	J/mol×K	680.40	Joback Method

cpg	442.42	J/mol×K	713.02	Joback Method
cpg	453.44	J/mol×K	745.63	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=C51755852&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