3-(acetylthio)hexyl acetate

Inchi: InChI=1S/C10H18O3S/c1-4-5-10(14-9(3)12)6-7-13-8(2)11/h10H,4-7H2,1-3H3
InchiKey: GSJSVAFGVJLTNQ-UHFFFAOYSA-N
Formula: C10H18O3S
SMILES: CCCC(CCOC(C)=O)SC(C)=O
Mol. weight [g/mol]: 218.31

Physical Properties

Property code	Value	Unit	Source
gf	-298.84	kJ/mol	Joback Method
hf	-570.52	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.388		Crippen Method
mcvol	177.120	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
ripol	1947.00		NIST Webbook
ripol	1947.00		NIST Webbook
tb	626.70	K	Joback Method
tc	827.31	K	Joback Method
tf	343.95	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.38	J/mol×K	626.70	Joback Method
cpg	459.18	J/mol×K	660.14	Joback Method
cpg	472.25	J/mol×K	693.57	Joback Method
cpg	484.61	J/mol×K	727.01	Joback Method
cpg	496.26	J/mol×K	760.44	Joback Method
cpg	507.19	J/mol×K	793.88	Joback Method
cpg	517.41	J/mol×K	827.31	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=R317621&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