3-(Acetylthio)-2-methylpentanal

Inchi: InChI=1S/C8H14O2S/c1-4-8(6(2)5-9)11-7(3)10/h5-6,8H,4H2,1-3H3
InchiKey: SHIMCASOQRNQSL-UHFFFAOYSA-N
Formula: C8H14O2S
SMILES: CCC(SC(C)=O)C(C)C=O
Mol. weight [g/mol]: 174.26

Physical Properties

Property code	Value	Unit	Source
gf	-183.72	kJ/mol	Joback Method
hf	-375.30	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.880		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1209.00		NIST Webbook
rinpol	1213.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	552.87	K	Joback Method
tc	761.12	K	Joback Method
tf	276.25	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.69	J/mol×K	552.87	Joback Method
cpg	339.13	J/mol×K	587.58	Joback Method
cpg	350.91	J/mol×K	622.29	Joback Method
cpg	362.04	J/mol×K	657.00	Joback Method
cpg	372.53	J/mol×K	691.71	Joback Method

cpg	382.40	J/mol×K	726.42	Joback Method
cpg	391.65	J/mol×K	761.12	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=R341852&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume