3-(Acetylthio)-2-ethylhexanal

Inchi: InChI=1S/C10H18O2S/c1-4-6-10(13-8(3)12)9(5-2)7-11/h7,9-10H,4-6H2,1-3H3
InchiKey: GANMVCGGCRYFKR-UHFFFAOYSA-N
Formula: C10H18O2S
SMILES: CCCC(SC(C)=O)C(C=O)CC
Mol. weight [g/mol]: 202.31

Physical Properties

Property code	Value	Unit	Source
gf	-166.88	kJ/mol	Joback Method
hf	-416.58	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.660		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1368.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	598.63	K	Joback Method
tc	800.64	K	Joback Method
tf	298.79	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.99	J/mol×K	598.63	Joback Method
cpg	435.02	J/mol×K	632.30	Joback Method
cpg	448.30	J/mol×K	665.97	Joback Method
cpg	460.85	J/mol×K	699.63	Joback Method
cpg	472.67	J/mol×K	733.30	Joback Method
cpg	483.79	J/mol×K	766.97	Joback Method

cpg	494.22	J/mol×K	800.64	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=R341847&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