

# 3-(Acetylthio)-2-butyloctanal

<b>Inchi:</b>	InChI=1S/C14H26O2S/c1-4-6-8-10-14(17-12(3)16)13(11-15)9-7-5-2/h11,13-14H,4-10H2
<b>InchiKey:</b>	AFHGFCHRYDRJRA-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O2S
<b>SMILES:</b>	CCCCC(SC(C)=O)C(C=O)CCCC
<b>Mol. weight [g/mol]:</b>	258.42

## Physical Properties

Property code	Value	Unit	Source
gf	-133.20	kJ/mol	Joback Method
hf	-499.14	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	66.27	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.220		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
ripol	1726.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2260.00		NIST Webbook
tb	690.15	K	Joback Method
tc	882.86	K	Joback Method
tf	343.87	K	Joback Method
vc	0.884	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.01	J/molxK	690.15	Joback Method
cpg	644.12	J/molxK	722.27	Joback Method
cpg	659.35	J/molxK	754.39	Joback Method
cpg	673.72	J/molxK	786.50	Joback Method
cpg	687.25	J/molxK	818.62	Joback Method

cpg	699.97	J/mol×K	850.74	Joback Method
cpg	711.89	J/mol×K	882.86	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R341832&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R341832&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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