

# Butanethioic acid, 3-oxo-, S-(1,1-dimethylethyl) ester

**Other names:** Acetoacetic acid, 1-thio-, S-tert-butyl ester

S-tert-Butyl 3-oxothiobutyrate

S-tert-Butyl acetothioacetate

tert-Butyl acetothiolacetate

**Inchi:** InChI=1S/C8H14O2S/c1-6(9)5-7(10)11-8(2,3)4/h5H2,1-4H3

**InchiKey:** FXOMETKMHQLOHH-UHFFFAOYSA-N

**Formula:** C8H14O2S

**SMILES:** CC(=O)CC(=O)SC(C)(C)C

**Mol. weight [g/mol]:** 174.26

**CAS:** 15925-47-0

## Physical Properties

Property code	Value	Unit	Source
gf	-205.40	kJ/mol	Joback Method
hf	-400.49	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.024		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	555.73	K	Joback Method
tc	772.83	K	Joback Method
tf	316.60	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.41	J/molxK	555.73	Joback Method
cpg	341.32	J/molxK	591.91	Joback Method
cpg	353.42	J/molxK	628.10	Joback Method
cpg	364.73	J/molxK	664.28	Joback Method
cpg	375.30	J/molxK	700.46	Joback Method

cpg	385.15	J/mol×K	736.64	Joback Method
cpg	394.32	J/mol×K	772.83	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	0.10	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15925470&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15925470&amp;Units=SI</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>hvap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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