

# Butanoic acid, 4-([4h, 5h]thiazol-2-ylthio)-, ethyl ester

Inchi:	InChI=1S/C9H15NO2S2/c1-2-12-8(11)4-3-6-13-9-10-5-7-14-9/h2-7H2,1H3
InchiKey:	OGADGLVDONULII-UHFFFAOYSA-N
Formula:	C9H15NO2S2
SMILES:	CCOC(=O)CCCSC1=NCCS1
Mol. weight [g/mol]:	233.35
CAS:	22623-65-0

## Physical Properties

Property code	Value	Unit	Source
gf	45.33	kJ/mol	Joback Method
hf	-188.66	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.166		Crippen Method
mcvol	172.630	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	676.01	K	Joback Method
tc	916.47	K	Joback Method
tf	481.16	K	Joback Method
vc	0.640	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.23	J/molxK	676.01	Joback Method
cpg	466.25	J/molxK	716.09	Joback Method
cpg	480.17	J/molxK	756.16	Joback Method
cpg	492.98	J/molxK	796.24	Joback Method
cpg	504.69	J/molxK	836.32	Joback Method
cpg	515.29	J/molxK	876.40	Joback Method
cpg	524.79	J/molxK	916.47	Joback Method

# Sources

<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=C22623650&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22623650&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/38-950-5/Butanoic-acid-4-4h-5h-thiazol-2-ylthio-ethyl-ester.pdf>

Generated by Cheméo on 2024-05-06 19:23:50.074187096 +0000 UTC m=+17312678.994764413.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.