

# 1,3-diethyl-2-thiobarbituric acid

<b>Other names:</b>	1,3-diethyl-2-thioxodihydropyrimidine-4,6(1H,5H)-dione
<b>Inchi:</b>	InChI=1S/C8H12N2O2S/c1-3-9-6(11)5-7(12)10(4-2)8(9)13/h3-5H2,1-2H3
<b>InchiKey:</b>	SHBTUGJAKBRBBJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H12N2O2S
<b>SMILES:</b>	CCN1C(=O)CC(=O)N(CC)C1=S
<b>Mol. weight [g/mol]:</b>	200.26

## Physical Properties

Property code	Value	Unit	Source
hfus	35.50 ± 0.50	kJ/mol	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
log10ws	-1.10		Crippen Method
logp	0.372		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
tt	377.10 ± 0.20	K	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	282.30 ± 8.90	J/mol×K	360.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	213.50 ± 2.60	J/mol×K	265.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry

cps	217.30 ± 2.50	J/mol×K	270.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	219.80 ± 2.30	J/mol×K	273.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	221.20 ± 2.50	J/mol×K	275.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	224.50 ± 2.10	J/mol×K	280.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	227.70 ± 2.00	J/mol×K	285.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	230.40 ± 2.20	J/mol×K	290.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	233.70 ± 2.50	J/mol×K	295.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	236.90 ± 2.10	J/mol×K	298.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	287.20 ± 9.30	J/mol×K	365.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry

cps	240.80 ± 2.60	J/mol×K	305.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	244.80 ± 3.30	J/mol×K	310.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	249.80 ± 4.60	J/mol×K	315.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	252.90 ± 4.90	J/mol×K	320.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	256.10 ± 7.30	J/mol×K	325.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	259.70 ± 7.50	J/mol×K	330.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	263.10 ± 7.70	J/mol×K	335.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	266.50 ± 8.00	J/mol×K	340.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry

cps	269.70 ± 7.60	J/mol×K	345.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	273.30 ± 8.30	J/mol×K	350.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	277.80 ± 8.40	J/mol×K	355.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
cps	238.90 ± 3.10	J/mol×K	300.15	Thermophysical Study of 2-Thiobarbituric Acids by Differential Scanning Calorimetry
psub	0.03	kPa	375.90	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	3.90e-04	kPa	327.30	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	7.40e-04	kPa	333.60	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study

psub	1.10e-03	kPa	337.70	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	1.35e-03	kPa	340.00	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	1.85e-03	kPa	343.00	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	2.93e-03	kPa	348.00	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	3.40e-03	kPa	349.10	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	3.84e-03	kPa	351.00	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	4.89e-03	kPa	353.30	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study

psub	5.51e-03	kPa	354.10	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	6.34e-03	kPa	355.30	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	7.56e-03	kPa	358.10	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	0.01	kPa	362.40	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	0.02	kPa	367.70	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	0.02	kPa	368.60	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	0.02	kPa	370.70	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study

psub	0.03	kPa	372.20	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
psub	0.04	kPa	375.70	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study
rhos	1610.00	kg/m3	293.00	Thermochemistry of 1,3-diethylbarbituric and 1,3-diethyl-2-thiobarbituric acids: Experimental and computational study

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Thermochemistry of

<https://www.doi.org/10.1016/j.jct.2014.06.001>

1,3-diethylbarbituric and

1,3-diethyl-2-thiobarbituric acids:

<https://www.doi.org/10.1021/je200420u>

Experimental and Computational Study:

<http://link.springer.com/article/10.1007/BF02311772>

McGowan Characteristic Volume:

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

## Legend

<b>cps:</b>	Solid phase heat capacity
<b>hfus:</b>	Enthalpy of fusion 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>psub:</b>	Sublimation pressure
<b>rhos:</b>	Solid Density
<b>tt:</b>	Triple Point Temperature

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