

# 3H-1,2-Benzodithiole-3-thione

**Inchi:** InChI=1S/C7H4S3/c8-7-5-3-1-2-4-6(5)9-10-7/h1-4H  
**InchiKey:** MIGJSZGTFNIFSCC-UHFFFAOYSA-N  
**Formula:** C7H4S3  
**SMILES:** S=c1ssc2ccccc12  
**Mol. weight [g/mol]:** 184.30  
**CAS:** 3354-42-5

## Physical Properties

Property code	Value	Unit	Source
chs	-5276.00 ± 5.00	kJ/mol	NIST Webbook
hf	251.00	kJ/mol	NIST Webbook
hfs	144.00 ± 5.00	kJ/mol	NIST Webbook
hsub	107.00 ± 0.40	kJ/mol	NIST Webbook
hsub	107.00	kJ/mol	NIST Webbook
hsub	107.00	kJ/mol	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-3.64		Crippen Method
logp	3.692		Crippen Method
mcvol	119.620	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	102.60 ± 0.40	kJ/mol	355.50	NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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