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: MIGJSZGTNIFSCC-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/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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