4,5-Tetramethylene-1,2-dithiol-3-thione

Inchi: InChI=1S/C7H8S3/c8-7-5-3-1-2-4-6(5)9-10-7/h1-4H2
InchiKey: WNPWNYMVKHOGRA-UHFFFAOYSA-N
Formula: C7H8S3
SMILES: S=c1ssc2c1CCCC2
Mol. weight [g/mol]: 188.33
CAS: 14085-34-8

Physical Properties

Property code	Value	Unit	Source
chs	-5754.30 ± 8.40	kJ/mol	NIST Webbook
hf	156.00	kJ/mol	NIST Webbook
hfs	50.20 ± 8.40	kJ/mol	NIST Webbook
hsub	105.30	kJ/mol	NIST Webbook
hsub	105.30	kJ/mol	NIST Webbook
hsub	105.80	kJ/mol	NIST Webbook
log10ws	-3.34		Crippen Method
logp	3.418		Crippen Method
mcvol	128.220	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	101.60	kJ/mol	342.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14085348&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume