

1,3-Dithiole-2-thione

Other names:	1,3-Dithiol-2-thione Vinylene trithiocarbonate 1,3-Dithiacyclopentane, 2-thione-
Inchi:	InChI=1S/C3H2S3/c4-3-5-1-2-6-3/h1-2H
InchiKey:	WYKJWNVWJOKVQP-UHFFFAOYSA-N
Formula:	C3H2S3
SMILES:	S=c1sccs1
Mol. weight [g/mol]:	134.24
CAS:	930-35-8

Physical Properties

Property code	Value	Unit	Source
chs	-3441.00 ± 6.70	kJ/mol	NIST Webbook
hf	253.00 ± 6.70	kJ/mol	NIST Webbook
hsub	75.40 ± 0.40	kJ/mol	NIST Webbook
hsub	85.40 ± 0.40	kJ/mol	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	2.539		Crippen Method
mvol	82.720	ml/mol	McGowan Method

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=C930358&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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