

[1,3]DITHIANE-2-THIONE

Other names:	1,3-Dithian-2-thione m-Dithiane-2-thione Carbonic acid, trithio-, cyclic trimethylene ester Trimethylene trithiocarbonate 1,3-Dithiacyclohexane-2-thione 1,3-Propanedithiol, cyclic carbonotrithioate 1,3-Propanedithiol, cyclic trithioacarbonate
Inchi:	InChI=1S/C4H6S3/c5-4-6-2-1-3-7-4/h1-3H2
InchiKey:	BVNLWJVULAZODX-UHFFFAOYSA-N
Formula:	C4H6S3
SMILES:	S=C1SCCCS1
Mol. weight [g/mol]:	150.29

Physical Properties

Property code	Value	Unit	Source
chg	-4224.60 ± 0.40	kJ/mol	NIST Webbook
hf	77.50 ± 2.70	kJ/mol	NIST Webbook
hfus	10.23	kJ/mol	Joback Method
hsub	91.40 ± 2.50	kJ/mol	NIST Webbook
hsub	91.40 ± 2.50	kJ/mol	NIST Webbook
hvap	91.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
logp	2.141		Crippen Method
mcvol	101.110	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.99	J/mol×K	483.44	Joback Method
cpg	184.01	J/mol×K	529.10	Joback Method
cpg	193.10	J/mol×K	574.76	Joback Method
cpg	201.34	J/mol×K	620.41	Joback Method
cpg	208.82	J/mol×K	666.07	Joback Method

cpg	215.63	J/mol×K	711.73	Joback Method
cpg	221.85	J/mol×K	757.39	Joback Method
hsubt	88.60	kJ/mol	334.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1748158&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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