

4,5-Tetramethylene-1,3-dithiolanthione-2

Inchi:	InChI=1S/C7H10S3/c8-7-9-5-3-1-2-4-6(5)10-7/h5-6H,1-4H2
InchiKey:	FFIFYXTYVXGTRN-UHFFFAOYSA-N
Formula:	C7H10S3
SMILES:	S=C1SC2CCCCC2S1
Mol. weight [g/mol]:	190.35
CAS:	2164-87-6

Physical Properties

Property code	Value	Unit	Source
chs	-5911.57 ± 0.84	kJ/mol	NIST Webbook
gf	263.83	kJ/mol	Joback Method
hf	25.00	kJ/mol	NIST Webbook
hfus	17.20	kJ/mol	Joback Method
hsub	103.90 ± 2.90	kJ/mol	NIST Webbook
hsub	104.00 ± 3.00	kJ/mol	NIST Webbook
hvap	50.62	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.062		Crippen Method
mcvol	132.520	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	554.15	K	Joback Method
tc	831.83	K	Joback Method
tf	424.54	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.39	J/molxK	554.15	Joback Method
cpg	301.48	J/molxK	600.43	Joback Method
cpg	315.17	J/molxK	646.71	Joback Method
cpg	327.62	J/molxK	692.99	Joback Method
cpg	338.97	J/molxK	739.27	Joback Method
cpg	349.37	J/molxK	785.55	Joback Method

cpg	358.99	J/mol×K	831.83	Joback Method
hsubt	99.00	kJ/mol	361.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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