

# 1,4,6,9-Tetrathiaspiro[4.4]nonane

<b>Other names:</b>	Orthocarbonic acid, tetrathio-, cyclic diethylene ester
<b>Inchi:</b>	InChI=1S/C5H8S4/c1-2-7-5(6-1)8-3-4-9-5/h1-4H2
<b>InchiKey:</b>	OIXFQRVSKVDFW-UHFFFAOYSA-N
<b>Formula:</b>	C5H8S4
<b>SMILES:</b>	C1CSC2(S1)SCCS2
<b>Mol. weight [g/mol]:</b>	196.38
<b>CAS:</b>	13145-46-5

## Physical Properties

Property code	Value	Unit	Source
gf	238.08	kJ/mol	Joback Method
hf	197.21	kJ/mol	Joback Method
hfus	5.93	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
ie	8.26	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	-2.84		Crippen Method
logp	2.558		Crippen Method
mcvol	124.990	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	536.32	K	Joback Method
tc	849.54	K	Joback Method
tf	533.37	K	Joback Method
vc	0.389	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.06	J/molxK	536.32	Joback Method
cpg	263.46	J/molxK	588.52	Joback Method
cpg	275.25	J/molxK	640.73	Joback Method
cpg	285.87	J/molxK	692.93	Joback Method
cpg	295.75	J/molxK	745.14	Joback Method
cpg	305.35	J/molxK	797.34	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13145465&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13145465&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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