

# 1,5,7,11-Tetrathiaspiro[5.5]undecane

<b>Inchi:</b>	InChI=1S/C7H12S4/c1-3-8-7(9-4-1)10-5-2-6-11-7/h1-6H2
<b>InchiKey:</b>	LZGXFMIPVMFXAQ-UHFFFAOYSA-N
<b>Formula:</b>	C7H12S4
<b>SMILES:</b>	C1CSC2(SC1)SCCS2
<b>Mol. weight [g/mol]:</b>	224.43
<b>CAS:</b>	180-97-2

## Physical Properties

Property code	Value	Unit	Source
gf	230.72	kJ/mol	Joback Method
hf	143.61	kJ/mol	Joback Method
hfus	6.92	kJ/mol	Joback Method
hvap	54.27	kJ/mol	Joback Method
ie	8.09	eV	NIST Webbook
log10ws	-3.67		Crippen Method
logp	3.338		Crippen Method
mccvol	153.170	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	590.62	K	Joback Method
tc	911.27	K	Joback Method
tf	548.87	K	Joback Method
vc	0.484	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.79	J/molxK	590.62	Joback Method
cpg	357.65	J/molxK	644.06	Joback Method
cpg	373.83	J/molxK	697.50	Joback Method
cpg	388.76	J/molxK	750.94	Joback Method
cpg	402.88	J/molxK	804.38	Joback Method
cpg	416.65	J/molxK	857.82	Joback Method
cpg	430.49	J/molxK	911.27	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C180972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C180972&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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

Latest version available from:

<https://www.cheméo.com/cid/50-686-5/1-5-7-11-Tetrathiaspiro-5-5-undecane.pdf>

Generated by Cheméo on 2024-04-30 06:35:46.968367097 +0000 UTC m=+16748195.888944417.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.