

# Thiirane,cis-2,3-diethynyl-

<b>Inchi:</b>	InChI=1S/C6H4S/c1-3-5-6(4-2)7-5/h1-2,5-6H/t5-,6+
<b>InchiKey:</b>	ZEODDVBXGCQFTC-OLQVQODUSA-N
<b>Formula:</b>	C6H4S
<b>SMILES:</b>	C#CC1SC1C#C
<b>Mol. weight [g/mol]:</b>	108.16
<b>CAS:</b>	50555-56-1

## Physical Properties

Property code	Value	Unit	Source
gf	538.68	kJ/mol	Joback Method
hf	514.35	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	34.08	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	0.737		Crippen Method
mcvol	83.690	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	366.82	K	Joback Method
tc	594.35	K	Joback Method
tf	348.47	K	Joback Method
vc	0.297	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.44	J/molxK	366.82	Joback Method
cpg	148.35	J/molxK	404.74	Joback Method
cpg	156.51	J/molxK	442.66	Joback Method
cpg	163.97	J/molxK	480.59	Joback Method
cpg	170.79	J/molxK	518.51	Joback Method
cpg	177.02	J/molxK	556.43	Joback Method
cpg	182.73	J/molxK	594.35	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=C50555561&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50555561&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>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</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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