

# Thianthrene, 5-oxide

<b>Other names:</b>	Thianthrene monooxide Thianthrene oxide Thianthrene S-oxide
<b>Inchi:</b>	InChI=1S/C12H8OS2/c13-15-11-7-3-1-5-9(11)14-10-6-2-4-8-12(10)15/h1-8H
<b>InchiKey:</b>	NYVGTLXTOJKHJN-UHFFFAOYSA-N
<b>Formula:</b>	C12H8OS2
<b>SMILES:</b>	O=S1c2ccccc2Sc2ccccc21
<b>Mol. weight [g/mol]:</b>	232.32
<b>CAS:</b>	2362-50-7

## Physical Properties

Property code	Value	Unit	Source
gf	165.17	kJ/mol	Joback Method
hf	101.32	kJ/mol	Joback Method
hfus	24.24	kJ/mol	Joback Method
hvap	65.77	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.318		Crippen Method
mcvol	160.130	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	629.58	K	Joback Method
tc	899.25	K	Joback Method
tf	407.70 ± 1.00	K	NIST Webbook
vc	0.586	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.27	J/mol×K	629.58	Joback Method
cpg	373.47	J/mol×K	674.53	Joback Method
cpg	385.38	J/mol×K	719.47	Joback Method
cpg	396.16	J/mol×K	764.42	Joback Method
cpg	405.99	J/mol×K	809.36	Joback Method
cpg	415.00	J/mol×K	854.31	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2362507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2362507&amp;Units=SI</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>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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