

# 2-Methyl-5-phenyl-6a-thiathiophthene

<b>Inchi:</b>	InChI=1S/C12H10S3/c1-9-7-11-8-12(14-15(11)13-9)10-5-3-2-4-6-10/h2-8H,1H3
<b>InchiKey:</b>	PLHURWKLJVJSMF-UHFFFAOYSA-N
<b>Formula:</b>	C12H10S3
<b>SMILES:</b>	CC1=CC2=S(S1)SC(c1ccccc1)=C2
<b>Mol. weight [g/mol]:</b>	250.40
<b>CAS:</b>	1016-98-4

## Physical Properties

Property code	Value	Unit	Source
gf	388.50	kJ/mol	Joback Method
hf	309.49	kJ/mol	Joback Method
hfus	21.98	kJ/mol	Joback Method
hvap	65.67	kJ/mol	Joback Method
ie	7.43	eV	NIST Webbook
log10ws	-5.82		Crippen Method
logp	4.696		Crippen Method
mcvol	174.910	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	689.03	K	Joback Method
tc	990.51	K	Joback Method
tf	562.18	K	Joback Method
vc	0.612	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.68	J/molxK	689.03	Joback Method
cpg	421.17	J/molxK	739.28	Joback Method
cpg	434.26	J/molxK	789.52	Joback Method
cpg	446.10	J/molxK	839.77	Joback Method
cpg	456.86	J/molxK	890.02	Joback Method
cpg	466.68	J/molxK	940.26	Joback Method
cpg	475.73	J/molxK	990.51	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=C1016984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016984&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>h vap:</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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