

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

<b>Inchi:</b>	InChI=1S/C12H10S4/c1-13-12-8-10-7-11(14-16(10)15-12)9-5-3-2-4-6-9/h2-8H,1H3
<b>InchiKey:</b>	UGMZZSWLNLHKR-UHFFFAOYSA-N
<b>Formula:</b>	C12H10S4
<b>SMILES:</b>	CSC1=CC2=S(S1)SC(c1ccccc1)=C2
<b>Mol. weight [g/mol]:</b>	282.47
<b>CAS:</b>	20365-77-9

## Physical Properties

Property code	Value	Unit	Source
gf	421.62	kJ/mol	Joback Method
hf	351.36	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
ie	7.24	eV	NIST Webbook
log10ws	-6.20		Crippen Method
logp	4.997		Crippen Method
mcvol	191.260	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	757.81	K	Joback Method
tc	1076.78	K	Joback Method
tf	596.58	K	Joback Method
vc	0.665	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.58	J/molxK	757.81	Joback Method
cpg	466.23	J/molxK	810.97	Joback Method
cpg	478.41	J/molxK	864.13	Joback Method
cpg	489.27	J/molxK	917.29	Joback Method
cpg	498.99	J/molxK	970.46	Joback Method
cpg	507.71	J/molxK	1023.62	Joback Method
cpg	515.61	J/molxK	1076.78	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=C20365779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20365779&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>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.chemeo.com/cid/24-303-8/2-Methylthio-5-phenyl-6a-thiathiophthene.pdf>

Generated by Cheméo on 2024-05-03 11:34:10.084969913 +0000 UTC m=+17025299.005547225.

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