

# Pentakis(methylthio)benzene

<b>Inchi:</b>	InChI=1S/C11H16S5/c1-12-7-6-8(13-2)10(15-4)11(16-5)9(7)14-3/h6H,1-5H3
<b>InchiKey:</b>	SYAFJBVKTONLAY-UHFFFAOYSA-N
<b>Formula:</b>	C11H16S5
<b>SMILES:</b>	CSc1cc(SC)c(SC)c(SC)c1SC
<b>Mol. weight [g/mol]:</b>	308.57
<b>CAS:</b>	65516-74-7

## Physical Properties

Property code	Value	Unit	Source
gf	281.23	kJ/mol	Joback Method
hf	129.63	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	79.09	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	5.296		Crippen Method
mcvol	223.840	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	841.58	K	Joback Method
tc	1133.61	K	Joback Method
tf	462.23	K	Joback Method
vc	0.814	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.76	J/molxK	841.58	Joback Method
cpg	567.38	J/molxK	890.25	Joback Method
cpg	578.19	J/molxK	938.92	Joback Method
cpg	587.12	J/molxK	987.60	Joback Method
cpg	594.11	J/molxK	1036.27	Joback Method
cpg	599.08	J/molxK	1084.94	Joback Method
cpg	601.99	J/molxK	1133.61	Joback Method

# Sources

<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=C65516747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C65516747&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.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>

# 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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