

# 3,4-Dimethoxythiophenol

<b>Inchi:</b>	InChI=1S/C8H10O2S/c1-9-7-4-3-6(11)5-8(7)10-2/h3-5,11H,1-2H3
<b>InchiKey:</b>	MTKAJLNGIVXZIS-UHFFFAOYSA-N
<b>Formula:</b>	C8H10O2S
<b>SMILES:</b>	COc1ccc(S)cc1OC
<b>Mol. weight [g/mol]:</b>	170.23
<b>CAS:</b>	700-96-9

## Physical Properties

Property code	Value	Unit	Source
gf	-70.98	kJ/mol	Joback Method
hf	-220.82	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	48.56	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.992		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	526.78	K	Joback Method
tc	758.79	K	Joback Method
tf	312.30	K	Joback Method
vc	0.466	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.42	J/molxK	526.78	Joback Method
cpg	277.34	J/molxK	565.45	Joback Method
cpg	288.71	J/molxK	604.12	Joback Method
cpg	299.51	J/molxK	642.79	Joback Method
cpg	309.73	J/molxK	681.45	Joback Method
cpg	319.36	J/molxK	720.12	Joback Method
cpg	328.37	J/molxK	758.79	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=C700969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C700969&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>
<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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