

# Benzene, 5-isothiocyanato-1,2,3-trimethoxy-

<b>Other names:</b>	3,4,5-Trimethoxyphenyl isothiocyanate
<b>Inchi:</b>	InChI=1S/C10H11NO3S/c1-12-8-4-7(11-6-15)5-9(13-2)10(8)14-3/h4-5H,1-3H3
<b>InchiKey:</b>	AFWKAIYTSPWWCA-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO3S
<b>SMILES:</b>	COc1cc(N=C=S)cc(OC)c1OC
<b>Mol. weight [g/mol]:</b>	225.26
<b>CAS:</b>	35967-24-9

## Physical Properties

Property code	Value	Unit	Source
hf	-160.20	kJ/mol	Joback Method
hvap	59.79	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.447		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	683.03	K	Joback Method
tc	922.37	K	Joback Method

## Sources

<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=C35967249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35967249&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>

## Legend

<b>hf:</b>	Enthalpy of formation 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

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