

# 3-Methoxycarbonylphenyl isothiocyanate

Inchi:	InChI=1S/C9H7NO2S/c1-12-9(11)7-3-2-4-8(5-7)10-6-13/h2-5H,1H3
InchiKey:	NQXFZEJJHPUMMF-UHFFFAOYSA-N
Formula:	C9H7NO2S
SMILES:	COC(=O)c1ccccc(N=C=S)c1
Mol. weight [g/mol]:	193.22
CAS:	3125-66-4

## Physical Properties

Property code	Value	Unit	Source
hf	35.24	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.208		Crippen Method
mcvol	139.080	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	659.22	K	Joback Method
tc	916.43	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3125664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3125664&amp;Units=SI</a>
<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>

## 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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