

# Thiophene, 2-methoxy 3,5-dinitro

<b>Inchi:</b>	InChI=1S/C5H4N2O5S/c1-12-5-3(6(8)9)2-4(13-5)7(10)11/h2H,1H3
<b>InchiKey:</b>	RJWFPSOMDHNPMZ-UHFFFAOYSA-N
<b>Formula:</b>	C5H4N2O5S
<b>SMILES:</b>	COc1sc([N+](=O)[O-])cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	204.16
<b>CAS:</b>	27357-00-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.573		Crippen Method
mcvol	118.910	ml/mol	McGowan 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=C27357002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27357002&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>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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<https://www.chemeo.com/cid/37-256-7/Thiophene-2-methoxy-3-5-dinitro.pdf>

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