

# 3-nitrothiophene

**Inchi:** InChI=1S/C4H3NO2S/c6-5(7)4-1-2-8-3-4/h1-3H  
**InchiKey:** SIPCFXFCVTUAID-UHFFFAOYSA-N  
**Formula:** C4H3NO2S  
**SMILES:** O=[N+]([O-])c1ccsc1  
**Mol. weight [g/mol]:** 129.14  
**CAS:** 822-84-4

## Physical Properties

Property code	Value	Unit	Source
ie	9.62	eV	NIST Webbook
ie	9.78	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.656		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
tb	498.20	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.60	NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C822844&Units=SI&Mask=3FFF>

# Legend

<b>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

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