

# 2-Methoxythiophene

<b>Other names:</b>	Thiophene, 2-methoxy-
<b>Inchi:</b>	InChI=1S/C5H6OS/c1-6-5-3-2-4-7-5/h2-4H,1H3
<b>InchiKey:</b>	OKEHURCMYKPVFW-UHFFFAOYSA-N
<b>Formula:</b>	C5H6OS
<b>SMILES:</b>	COc1cccs1
<b>Mol. weight [g/mol]:</b>	114.17
<b>CAS:</b>	16839-97-7

## Physical Properties

Property code	Value	Unit	Source
ie	8.02	eV	NIST Webbook
ie	8.14 ± 0.05	eV	NIST Webbook
ie	8.08	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.757		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
rinpol	878.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	0.13	kPa	278.10	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.16	kPa	281.00	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.18	kPa	283.00	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.23	kPa	285.90	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.27	kPa	287.80	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.32	kPa	290.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.39	kPa	292.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.46	kPa	295.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.54	kPa	297.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.64	kPa	300.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.70	kPa	302.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.87	kPa	305.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.99	kPa	307.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.15	kPa	310.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.34	kPa	312.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.30	kPa	312.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	1.37	kPa	313.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.56	kPa	315.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.83	kPa	318.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	2.20	kPa	321.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	2.47	kPa	323.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
---------------	-------	------	----------------	--------

## 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=C16839977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16839977&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>Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase:</b>	<a href="https://www.doi.org/10.1016/j.jct.2013.11.003">https://www.doi.org/10.1016/j.jct.2013.11.003</a>

## 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>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/19-613-0/2-Methoxythiophene.pdf>

Generated by Cheméo on 2024-04-29 20:01:11.701718621 +0000 UTC m=+16710120.622295936.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.