

Thiophene, 3-methoxy-

Other names:	3-methoxythiophene
Inchi:	InChI=1S/C5H6OS/c1-6-5-2-3-7-4-5/h2-4H,1H3
InchiKey:	RFSKGCVUDQRZSD-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	COc1ccsc1
Mol. weight [g/mol]:	114.17
CAS:	17573-92-1

Physical Properties

Property code	Value	Unit	Source
ie	8.19	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.757		Crippen Method
mvol	84.070	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	0.09	kPa	278.10	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.11	kPa	281.00	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.14	kPa	283.90	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.17	kPa	286.80	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.21	kPa	289.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.26	kPa	292.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.32	kPa	295.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.36	kPa	297.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.43	kPa	300.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.52	kPa	303.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.63	kPa	306.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	0.76	kPa	309.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

pvap	0.92	kPa	312.60	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.08	kPa	315.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.31	kPa	318.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.54	kPa	321.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase
pvap	1.76	kPa	324.70	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase: <https://www.doi.org/10.1016/j.jct.2013.11.003>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17573921&Units=SI>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure

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