2-Methoxythiophene

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

Physical Properties

Property code	Value	Unit	Source
ie	8.18	eV	NIST Webbook
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
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

tbrp	424.70	K	102.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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=C16839977&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
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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