2-Thiophenemethanol

Other names:	(thiophen-2-yl)methanol
	2-(hydroxymethyl)thiophene
	2-Hydroxymethylthiophene
	2-Thiophenecarbinol
	2-thenyl alcohol
	2-thienylcarbinol
	2-thienylmethanol
	Thiophene, 2-(hydroxymethyl)-
	Thiophene-2-methanol
Inchi:	InChI=1S/C5H6OS/c6-4-5-2-1-3-7-5/h1-3,6H,4H2
InchiKey:	ZPHGMBGIFODUMF-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	OCc1cccs1
Mol. weight [g/mol]:	114.17
CAS:	636-72-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	1.240		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1024.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1937.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1951.00		NIST Webbook
ripol	1937.00		NIST Webbook
tb	480.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	0.55	kPa	351.15	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	0.67	kPa	354.25	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	0.79	kPa	357.17	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.02	kPa	361.30	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.27	kPa	365.19	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.35	kPa	366.38	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

pvap	1.42	kPa	367.49	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.48	kPa	368.14	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.61	kPa	369.77	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.88	kPa	372.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	1.96	kPa	373.21	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	2.44	kPa	377.74	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	3.06	kPa	382.13	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

pvap	3.67	kPa	386.07	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	3.93	kPa	387.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	4.15	kPa	388.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	4.77	kPa	391.84	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	5.25	kPa	393.87	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	6.25	kPa	397.94	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	6.80	kPa	399.72	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	7.60	kPa	402.41	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	8.25	kPa	404.37	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	9.00	kPa	406.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	9.66	kPa	408.27	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	10.96	kPa	411.50	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	12.60	kPa	415.06	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	13.38	kPa	416.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

pvap	14.47	kPa	418.63	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	15.36	kPa	420.23	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	16.51	kPa	422.21	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	18.05	kPa	424.64	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	19.00	kPa	426.07	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	20.52	kPa	428.27	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	21.34	kPa	429.37	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	22.77	kPa	431.17	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	23.88	kPa	432.56	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	24.78	kPa	433.65	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.60	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling: https://www.doi.org/10.1016/j.jct.2017.07.008

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C636726&Units=SI

Legend

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure