3-Methyl-2-thiophenecarboxylic acid

Other names:	2-Thiophenecarboxylic acid, 3-methyl-
	3-Methylthiophene-2-carboxylic acid
	3-methyl-2-thenoic acid
	Methyl 2-thiophenecarboxylate
Inchi:	InChI=1S/C6H6O2S/c1-4-2-3-9-5(4)6(7)8/h2-3H,1H3,(H,7,8)
InchiKey:	IFLKEBSJTZGCJG-UHFFFAOYSA-N
Formula:	C6H6O2S
SMILES:	Cc1ccsc1C(=O)O
Mol. weight [g/mol]:	142.18
CAS:	23806-24-8

Physical Properties

Property code	Value	Unit	Source
hsub	98.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.755		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
ripol	2501.00		NIST Webbook
ripol	2501.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	96.70 ± 0.40	kJ/mol	323.00	NIST Webbook
pvap	3.14e-04	kPa	322.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.02e-04	kPa	312.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	1.02e-04	kPa	312.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.29e-04	kPa	314.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.30e-04	kPa	314.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.26e-04	kPa	314.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.64e-04	kPa	316.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.62e-04	kPa	316.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.59e-04	kPa	316.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.09e-04	kPa	318.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.05e-04	kPa	318.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.04e-04	kPa	318.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.64e-04	kPa	320.19	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.61e-04	kPa	320.19	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	2.54e-04	kPa	320.19	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	3.23e-04	kPa	322.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	3.20e-04	kPa	322.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.04e-04	kPa	312.13	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.12e-04	kPa	324.14	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.07e-04	kPa	324.14	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.18e-04	kPa	324.14	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	5.07e-04	kPa	326.18	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	5.03e-04	kPa	326.18	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	5.07e-04	kPa	326.18	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	6.36e-04	kPa	328.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	6.30e-04	kPa	328.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	6.30e-04	kPa	328.21	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	7.98e-04	kPa	330.15	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	7.86e-04	kPa	330.15	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	7.69e-04	kPa	330.15	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	9.84e-04	kPa	332.23	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	9.72e-04	kPa	332.23	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	9.40e-04	kPa	332.23	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.19e-03	kPa	334.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.17e-03	kPa	334.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.15e-03	kPa	334.20	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23806248&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical properties of three 2-thiophenecarboxylic acid derivatives:	https://www.doi.org/10.1016/j.jct.2008.04.013

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
ripol:	Polar retention indices