

2-Thiophenecarboxylic acid, 5-methyl-

Other names:	2-Carboxy-5-methylthiophene 2-Methyl-5-thiophenecarboxylic acid 5-Methyl-2-thiophenecarboxylic acid 5-Methyl-2-thiophenecarboxylic acid (keto form) 5-Methyl-2-thiophenecarboxylic acid 5-Methylthiophen-2-carboxylic acid 5-methylthiophene-2-carboxylic acid
Inchi:	InChI=1S/C6H6O2S/c1-4-2-3-5(9-4)6(7)8/h2-3H,1H3,(H,7,8)
InchiKey:	VCNGNQLPFHCODE-UHFFFAOYSA-N
Formula:	C6H6O2S
SMILES:	Cc1ccc(C(=O)O)s1
Mol. weight [g/mol]:	142.18
CAS:	1918-79-2

Physical Properties

Property code	Value	Unit	Source
hsub	101.90 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.755		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	100.40 ± 0.30	kJ/mol	327.00	NIST Webbook
pvap	3.41e-04	kPa	328.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	8.90e-05	kPa	316.29	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.13e-04	kPa	318.25	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.12e-04	kPa	318.25	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.10e-04	kPa	318.25	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.39e-04	kPa	320.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.39e-04	kPa	320.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.39e-04	kPa	320.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.83e-04	kPa	322.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.80e-04	kPa	322.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.80e-04	kPa	322.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.29e-04	kPa	324.24	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.26e-04	kPa	324.24	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	2.22e-04	kPa	324.24	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.73e-04	kPa	326.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.78e-04	kPa	326.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	2.76e-04	kPa	326.12	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	8.80e-05	kPa	316.29	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	3.56e-04	kPa	328.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	3.55e-04	kPa	328.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.41e-04	kPa	330.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.39e-04	kPa	330.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	4.27e-04	kPa	330.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	5.40e-04	kPa	332.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	5.39e-04	kPa	332.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

pvap	5.39e-04	kPa	332.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	7.00e-04	kPa	334.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	6.97e-04	kPa	334.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	6.90e-04	kPa	334.28	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	8.59e-04	kPa	336.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	8.55e-04	kPa	336.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	8.43e-04	kPa	336.22	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.05e-03	kPa	338.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.05e-03	kPa	338.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	1.03e-03	kPa	338.11	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives
pvap	9.00e-05	kPa	316.29	Thermochemical properties of three 2-thiophenecarboxylic acid derivatives

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices

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