

# 2-Thiophenecarboxylic acid

<b>Other names:</b>	.alpha.-thiophenecarboxylic acid 2-TCA 2-carboxythiophene 2-thenoic acid 2-thiophenic acid Thenoic acid Thiophene-2-carboxylic acid «alpha»-Thiophenecarboxylic acid
<b>Inchi:</b>	InChI=1S/C5H4O2S/c6-5(7)4-2-1-3-8-4/h1-3H,(H,6,7)
<b>InchiKey:</b>	QERYCTSHXKAMIS-UHFFFAOYSA-N
<b>Formula:</b>	C5H4O2S
<b>SMILES:</b>	O=C(O)c1cccs1
<b>Mol. weight [g/mol]:</b>	128.15
<b>CAS:</b>	527-72-0

## Physical Properties

Property code	Value	Unit	Source
ie	9.35	eV	NIST Webbook
ie	9.14 ± 0.05	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	1.446		Crippen Method
mcvol	85.640	ml/mol	McGowan Method
rinpol	1199.00		NIST Webbook
tb	533.20	K	NIST Webbook
tf	400.00 ± 2.00	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cps	153.78	J/mol×K	298.15	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins
hfust	21.00	kJ/mol	400.90	NIST Webbook
hsubt	96.90	kJ/mol	318.50	NIST Webbook
hsubt	97.10	kJ/mol	319.00	NIST Webbook

## Sources

Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins: NIST Webbook:

<https://www.doi.org/10.1016/j.tca.2017.06.024>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C527720&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

<b>cps:</b>	Solid phase heat capacity
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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