

# 2-Thiopheneacetic acid

<b>Other names:</b>	2-Thienylacetic acid Thiophene-2-acetic acid Thiopheneacetic acid
<b>Inchi:</b>	InChI=1S/C6H6O2S/c7-6(8)4-5-2-1-3-9-5/h1-3H,4H2,(H,7,8)
<b>InchiKey:</b>	SMJRBWINMFUUDS-UHFFFAOYSA-N
<b>Formula:</b>	C6H6O2S
<b>SMILES:</b>	O=C(O)Cc1cccs1
<b>Mol. weight [g/mol]:</b>	142.18
<b>CAS:</b>	1918-77-0

## Physical Properties

Property code	Value	Unit	Source
h <sub>fus</sub>	14.00	kJ/mol	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
h <sub>sub</sub>	97.50 ± 1.40	kJ/mol	NIST Webbook
log <sub>10</sub> w <sub>s</sub>	-1.13		Crippen Method
log <sub>p</sub>	1.375		Crippen Method
m <sub>cvol</sub>	99.730	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
h <sub>fust</sub>	14.00	kJ/mol	337.40	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
t <sub>brp</sub>	433.20	K	2.90	NIST Webbook

# Sources

Thermophysical properties of sulfur heterocycles: Thiane and thiophene  
McGowan's Method:

<https://www.doi.org/10.1016/j.tca.2005.11.024>

NIST Webbook:

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

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918770&Units=SI>

Crippen Method:

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

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

## Legend

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<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>tbrp:</b>	Boiling point at reduced pressure

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