

2-Thiopheneacetic acid

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

Physical Properties

Property code	Value	Unit	Source
hfus	14.00	kJ/mol	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hsub	97.50 ± 1.40	kJ/mol	NIST Webbook
log10ws	-1.13		Crippen Method
logp	1.375		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.00	kJ/mol	337.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	2.90	NIST Webbook

Sources

Thermophysical properties of sulfur
heterocycles: Thiane and thiophene
derivatives

McGowan's Method:

NIST Webbook:

Crippen Method:

Crippen Method:

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

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

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

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

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

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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