

3-Thiopheneacetic acid

Other names:	3-Thienylacetic acid Thiophene-3-acetic acid
Inchi:	InChI=1S/C6H6O2S/c7-6(8)3-5-1-2-9-4-5/h1-2,4H,3H2,(H,7,8)
InchiKey:	RCNOGGGBSSVMAS-UHFFFAOYSA-N
Formula:	C6H6O2S
SMILES:	O=C(O)Cc1ccsc1
Mol. weight [g/mol]:	142.18
CAS:	6964-21-2

Physical Properties

Property code	Value	Unit	Source
hfus	18.80	kJ/mol	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hsub	100.90 ± 1.90	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	18.80	kJ/mol	353.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6964212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives:	https://www.doi.org/10.1016/j.tca.2005.11.024

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

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