3-Thiopheneacetic acid, methyl ester

Other names:	Methyl 3-thiopheneacetate
	methyl 3-thienylacetate
Inchi:	InChI=1S/C7H8O2S/c1-9-7(8)4-6-2-3-10-5-6/h2-3,5H,4H2,1H3
InchiKey:	RZGRWVULDSXQSM-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	COC(=O)Cc1ccsc1
Mol. weight [g/mol]:	156.20
CAS:	58414-52-1

Physical Properties

Property code	Value	Unit	Source
cpl	250.60	J/mol×K	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hvap	60.90 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.464		Crippen Method
mcvol	113.820	ml/mol	McGowan Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58414521&Units=SI

Legend

cpl:	Liquid phase heat capacity
hvap:	Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume