2-Thiopheneacetic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C10H10O2S/c1-3-8(2)12-10(11)7-9-5-4-6-13-9/h1,4-6,8H,7H2,2H3
InchiKey: JMUSKSDCKWSWAQ-UHFFFAOYSA-N
Formula: C10H10O2S
SMILES: C#CC(C)OC(=O)Cc1cccs1
Mol. weight [g/mol]: 194.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	1.856		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299384&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.