

Thiazole, 5-ethenyl-4-(methoxycarbonyl)

Inchi: InChI=1S/C7H7NO2S/c1-3-5-6(7(9)10-2)8-4-11-5/h3-4H,1H2,2H3
InchiKey: YJHGYYBTCCJNSH-UHFFFAOYSA-N
Formula: C7H7NO2S
SMILES: C=Cc1scnc1C(=O)OC
Mol. weight [g/mol]: 169.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	1.573		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
rinpole	1328.00		NIST Webbook
rinpole	1328.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R594531&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/116-204-6/Thiazole-5-ethenyl-4-methoxycarbonyl.pdf>

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