Thiazole, acetyl-ethyl

Inchi: InChI=1S/C7H9NOS/c1-3-6-7(5(2)9)8-4-10-6/h4H,3H2,1-2H3
InchiKey: MLQBANLPAYVLSE-UHFFFAOYSA-N
Formula: C7H9NOS
SMILES: CCc1scnc1C(C)=O
Mol. weight [g/mol]: 155.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	1.908		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R125987&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.