2-ethylthienothiophene

Inchi: InChI=1S/C8H8S2/c1-2-7-3-6-4-9-5-8(6)10-7/h3-5H,2H2,1H3
InchiKey: LMJZOBUJCKKBRY-UHFFFAOYSA-N
Formula: C8H8S2
SMILES: CCc1cc2cscc2s1
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.525		Crippen Method
mcvol	121.660	ml/mol	McGowan Method
rinpol	1422.00		NIST Webbook
ripol	2012.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R189238&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
ripol: Polar retention indices