Thiophene, 2,4-diethyl

Other names: 2,4-Diethyl-thiophene
Inchi: InChI=1S/C8H12S/c1-3-7-5-8(4-2)9-6-7/h5-6H,3-4H2,1-2H3
InchiKey: DBTZOIMPUSTZCD-UHFFFAOYSA-N
Formula: C8H12S
SMILES: CCc1csc(CC)c1
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.873		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R258958&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices