Thiazole, 4,5-diethyl

Inchi: InChI=1S/C7H11NS/c1-3-6-7(4-2)9-5-8-6/h5H,3-4H2,1-2H3
InchiKey: IGMHDSLRWSOXOW-UHFFFAOYSA-N
Formula: C7H11NS
SMILES: CCc1ncsc1CC
Mol. weight [g/mol]: 141.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	2.268		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1463.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R317676&Units=SI
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

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