Thiophene, 5-ethyl-2,3-dimethyl

Other names: 5-Ethyl-2,3-dimethylthiophene
Inchi: InChI=1S/C8H12S/c1-4-8-5-6(2)7(3)9-8/h5H,4H2,1-3H3
InchiKey: WFOUEDZBEUPAPA-UHFFFAOYSA-N
Formula: C8H12S
SMILES: CCc1cc(C)c(C)s1
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.927		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1055.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1056.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41897&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