Thiophene, 2-ethenyl-5-methyl

Other names: 2-Methyl-5-vinylthiophene
Inchi: InChI=1S/C7H8S/c1-3-7-5-4-6(2)8-7/h3-5H,1H2,2H3
InchiKey: ZDSXWSYLVMUDHI-UHFFFAOYSA-N
Formula: C7H8S
SMILES: C=Cc1ccc(C)s1
Mol. weight [g/mol]: 124.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	2.700		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
rinpol	971.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	971.00		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=R41780&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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