Pyrazine, 2-(2-thienylmethyl)-3,6-dimethyl

Inchi: InChI=1S/C11H12N2S/c1-8-7-12-9(2)11(13-8)6-10-4-3-5-14-10/h3-5,7H,6H2,1-2H3
InchiKey: SQJIZBGBPAYXRH-UHFFFAOYSA-N
Formula: C11H12N2S
SMILES: Cc1cnc(C)c(Cc2cccs2)n1
Mol. weight [g/mol]: 204.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.746		Crippen Method
mcvol	158.940	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		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=R87914&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.