

Pyrazine, 2-(2-thienylmethyl)-3,5-dimethyl

Inchi:	InChI=1S/C11H12N2S/c1-8-7-12-11(9(2)13-8)6-10-4-3-5-14-10/h3-5,7H,6H2,1-2H3
InchiKey:	SSBSPEAASUFVHE-UHFFFAOYSA-N
Formula:	C11H12N2S
SMILES:	Cc1cnc(Cc2cccs2)c(C)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	1603.00		NIST Webbook

Sources

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=R87900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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<https://www.chemeo.com/cid/23-506-4/Pyrazine-2-2-thienylmethyl-3-5-dimethyl.pdf>

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