3-Methyl-5-(2-methylpentyl)-2-(phenylthio)pyrazin

Other names: Pyrazine, 3-methyl-5-(2-methylpentyl)-2-(phenylthio)
Inchi: InChI=1S/C17H22N2S/c1-4-8-13(2)11-15-12-18-17(14(3)19-15)20-16-9-6-5-7-10-16/h5-7
InchiKey: BZFHMSYLAQBAEK-UHFFFAOYSA-N
Formula: C17H22N2S
SMILES: CCCC(C)Cc1cnc(Sc2ccccc2)c(C)n1
Mol. weight [g/mol]: 286.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	4.915		Crippen Method
mcvol	239.180	ml/mol	McGowan Method
rinpol	2064.00		NIST Webbook
ripol	2669.00		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=R38573&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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