3-Methyl-5-(2-methylbutyl)-2-(phenylthio)pyrazine

Other names: Pyrazine, 3-methyl-5-(2-methylbutyl)-2-(phenylthio)
Inchi: InChI=1S/C16H20N2S/c1-4-12(2)10-14-11-17-16(13(3)18-14)19-15-8-6-5-7-9-15/h5-9,11
InchiKey: KUBFPNOYLUSORB-UHFFFAOYSA-N
Formula: C16H20N2S
SMILES: CCC(C)Cc1cnc(Sc2ccccc2)c(C)n1
Mol. weight [g/mol]: 272.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	4.525		Crippen Method
mcvol	225.090	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
ripol	2569.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38555&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
ripol: Polar retention indices

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