Pyrazine, 3-methyl-5-(1-methylethyl)-2-(phenylthio)

Other names: 5-isopropyl-3-methyl-2-(phenylthio)pyrazine
Inchi: InChI=1S/C14H16N2S/c1-10(2)13-9-15-14(11(3)16-13)17-12-7-5-4-6-8-12/h4-10H,1-3H3
InchiKey: RKONQZQNZFCZCE-UHFFFAOYSA-N
Formula: C14H16N2S
SMILES: Cc1nc(C(C)C)cnc1Sc1ccccc1
Mol. weight [g/mol]: 244.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.060		Crippen Method
mcvol	196.910	ml/mol	McGowan Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2375.00		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=R38662&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
ripol: Polar retention indices