

5-isobutyl-3-methyl-2-(phenylthio)pyrazine

Other names: Pyrazine, 3-methyl-5-(2-methylpropyl)-2-(phenylthio)
Inchi: InChI=1S/C15H18N2S/c1-11(2)9-13-10-16-15(12(3)17-13)18-14-7-5-4-6-8-14/h4-8,10-11
InchiKey: QTDXLQFIMOYMD-UHFFFAOYSA-N
Formula: C15H18N2S
SMILES: Cc1nc(CC(C)C)cnc1Sc1ccccc1
Mol. weight [g/mol]: 258.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	4.135		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
ripol	2452.00		NIST Webbook
ripol	2452.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38626&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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