

5-sec-butyl-3-methyl-2-(phenylthio)pyrazine

Other names: Pyrazine, 3-methyl-5-(1-methylpropyl)-2-(phenylthio)
Inchi: InChI=1S/C15H18N2S/c1-4-11(2)14-10-16-15(12(3)17-14)18-13-8-6-5-7-9-13/h5-11H,4H
InchiKey: XPLUYVZBRORHQB-UHFFFAOYSA-N
Formula: C15H18N2S
SMILES: CCC(C)c1cnc(Sc2ccccc2)c(C)n1
Mol. weight [g/mol]: 258.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	4.450		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
ripol	2430.00		NIST Webbook
ripol	2430.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38747&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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