2,5-dimethyl-3-(phenylethyl)pyrazine

Other names: 2-(2'-phenyl-ethyl)-3,6-dimethylpyrazine
Inchi: InChI=1S/C14H16N2/c1-11-10-15-12(2)14(16-11)9-8-13-6-4-3-5-7-13/h3-7,10H,8-9H2,1-
InchiKey: ZQHVNMBZTVKXCX-UHFFFAOYSA-N
Formula: C14H16N2
SMILES: Cc1cnc(C)c(CCc2ccccc2)n1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.879		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
rinpol	1685.00		NIST Webbook
ripol	2421.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221466&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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