2-methyl-5-(phenylethyl)pyrazine

Other names: 2-(2'-phenyl-ethyl)-5-methylpyrazine
Inchi: InChI=1S/C13H14N2/c1-11-9-15-13(10-14-11)8-7-12-5-3-2-4-6-12/h2-6,9-10H,7-8H2,1H
InchiKey: NNFMYTZFNHMMEL-UHFFFAOYSA-N
Formula: C13H14N2
SMILES: Cc1cnc(CCc2ccccc2)cn1
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.570		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
ripol	2380.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221515&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