2-(2'-phenyl-ethyl)-6-methylpyrazine

Inchi: InChI=1S/C13H14N2/c1-11-9-14-10-13(15-11)8-7-12-5-3-2-4-6-12/h2-6,9-10H,7-8H2,1H
InchiKey: BIMRFSBICVPLLY-UHFFFAOYSA-N
Formula: C13H14N2
SMILES: Cc1cncc(CCc2ccccc2)n1
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
ripol	2403.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R389770&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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