Benzhydryl pyrazine

Inchi: InChI=1S/C17H14N2/c1-3-7-14(8-4-1)17(15-9-5-2-6-10-15)16-13-18-11-12-19-16/h1-13,
InchiKey: NQJKHIJTEVVVKS-UHFFFAOYSA-N
Formula: C17H14N2
SMILES: c1ccc(C(c2ccccc2)c2cnccn2)cc1
Mol. weight [g/mol]: 246.31
CAS: 28217-87-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.657		Crippen Method
mcvol	199.070	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28217870&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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