

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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/90-196-5/Benzhydryl-pyrazine.pdf>

Generated by Cheméo on 2024-05-02 01:48:49.017678853 +0000 UTC m=+16903777.938256171.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.