Piperazine,1-benzyl-4-(2-pyridyl)-

Inchi: InChI=1S/C16H19N3/c1-2-6-15(7-3-1)14-18-10-12-19(13-11-18)16-8-4-5-9-17-16/h1-9H,
InchiKey: PPZUTXLPTNQOFF-UHFFFAOYSA-N
Formula: C16H19N3
SMILES: c1ccc(CN2CCN(c3ccccn3)CC2)cc1
Mol. weight [g/mol]: 253.34
CAS: 63980-42-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.404		Crippen Method
mcvol	207.860	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63980427&Units=SI

Legend

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