Piperazine, 1-phenethyl-4-(2-propynyl)-

Inchi: InChI=1S/C15H20N2/c1-2-9-16-11-13-17(14-12-16)10-8-15-6-4-3-5-7-15/h1,3-7H,8-14H2

InchiKey: VZYOHJKUGKPEKG-UHFFFAOYSA-N

Formula: C15H20N2

SMILES: C#CCN1CCN(CCc2ccccc2)CC1

Mol. weight [g/mol]: 228.33

CAS: 72955-79-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	1.480		Crippen Method
mcvol	198.950	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72955794&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