1H-2,5-Benzoxazocine, 3,4,5,6-tetrahydro-5-methyl-1-phenyl-

Other names: 1H-2,5-Benzoxazocine, 3,4,5,6-tetrahydro-5-methyl-1-phenyl-
Fenazoxine
3,4,5,6-Tetrahydro-5-methyl-2-phenyl-1H-2,5-benzoxazocine

Inchi: InChI=1S/C17H19NO/c1-18-11-12-19-17(14-7-3-2-4-8-14)16-10-6-5-9-15(16)13-18/h2-1

InchiKey: RGPDEAGGEXEMMM-UHFFFAOYSA-N

Formula: C17H19NO

SMILES: CN1CCOC(c2ccccc2)c2ccccc2C1

Mol. weight [g/mol]: 253.35

Physical Properties

Property code	Value	Unit	Source
logp	3.238		Crippen Method
mcvol	207.860	ml/mol	McGowan Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13669700&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices