

Morpheridine

Other names:

4-Piperidinecarboxylic acid, 1-[2-(4-morpholinyl)ethyl]-4-phenyl-, ethyl ester
Isonipetric acid, 1-(2-morpholinoethyl)-4-phenyl-, ethyl ester
Morpheridin
TA 1
1-(2-Morpholinoethyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester
Morpholinoethyl morpethidine

Inchi:

InChI=1S/C20H30N2O3/c1-2-25-19(23)20(18-6-4-3-5-7-18)8-10-21(11-9-20)12-13-22-14

InchiKey:

JDEDMCKQPKGSAX-UHFFFAOYSA-N

Formula:

C20H30N2O3

SMILES:

CCOC(=O)C1(c2ccccc2)CCN(CCN2CCOCC2)CC1

Mol. weight [g/mol]:

346.46

CAS:

469-81-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	1.916		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
rinpole	2535.00		NIST Webbook
rinpole	2535.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C469818&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/120-848-7/Morpheridine.pdf>

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