

1-Piperidinepropanol, «alpha»-cyclopentyl-«alpha»-phenyl-

Other names:

Cycrimine

Pagitane

«alpha»-Cyclopentyl-«alpha»-phenyl-1-piperidinepropanol

Inchi:

InChI=1S/C19H29NO/c21-19(18-11-5-6-12-18,17-9-3-1-4-10-17)13-16-20-14-7-2-8-15-2

InchiKey:

SWRUZBWLEWHWRI-UHFFFAOYSA-N

Formula:

C19H29NO

SMILES:

OC(CCN1CCCCC1)(c1ccccc1)C1CCCC1

Mol. weight [g/mol]:

287.44

CAS:

77-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.940		Crippen Method
mcvol	248.940	ml/mol	McGowan Method
rinpol	2132.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2114.00		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=C77394&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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