1,5-Pentanediamine, N-(6-methoxy-8-quinolinyl)-N'-(1-methylethyl)-

Other names: Pentaquine
8-(5-Isopropylaminoamylamino)-6-methoxyquinoline
Pentaquin

Inchi: InChI=1S/C18H27N3O/c1-14(2)19-9-5-4-6-10-20-17-13-16(22-3)12-15-8-7-11-21-18(15)

InchiKey: VKXQZROIIKPELG-UHFFFAOYSA-N

Formula: C18H27N3O

SMILES: COc1cc(NCCCCCNC(C)C)c2ncccc2c1

Mol. weight [g/mol]: 301.43

CAS: 86-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	3.824		Crippen Method
mcvol	257.070	ml/mol	McGowan Method
rinpol	2540.00		NIST Webbook
rinpol	2555.00		NIST Webbook

Sources

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=C86782&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices