

# 1,5-Pentanediamine, N-(6-methoxy-8-quinoliny)-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(NCCCCNC(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:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C86782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86782&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## 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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