Isoquinoline, 1-[(3,4-diethoxyphenyl)methyl]-6,7-diethoxy-

Other names: Isoquinoline, 1-(3,4-diethoxybenzyl)-6,7-diethoxy-
Barbonin
Barbonine
6,7-Diaethoxy-1-(3,4-diaethoxybenzyl)isochinolin
1-(3,4-Diethoxybenzyl)-6,7-diethoxyisoquinoline
6,7-Diethoxy-1-(3,4-diethoxybenzyl)isoquinoline
Dyscural
Ethaverine
Ethylpapaverine
Isoquinoline, 6,7-diethoxy-1-(3,4-diethoxybenzyl)-
Perparine
Perperine

Inchi: InChI=1S/C24H29NO4/c1-5-26-21-10-9-17(14-22(21)27-6-2)13-20-19-16-24(29-8-4)23(2

InchiKey: ZOWYFYXTIWQBEP-UHFFFAOYSA-N

Formula: C24H29NO4

SMILES: CCOc1ccc(Cc2nccc3cc(OCC)c(OCC)cc23)cc1OCC

Mol. weight [g/mol]: 395.49

CAS: 486-47-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	5.420		Crippen Method
mcvol	315.500	ml/mol	McGowan Method
rinpol	2945.00		NIST Webbook
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
rinpol	2975.00		NIST Webbook

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C486475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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