4-DIPHENYLMETHOXY-1-METHYLPIPERIDINE

Other names: Piperidine, 4-(diphenylmethoxy)-1-methyl-
AN 1041
Belfene
Dayfen
Diphenylpyrilene
Hispril
Histryl
Histyn
Hystryl
Lyssipoll
Mepiben
N-Methyl-4-(Benzhydryloxy)piperidine
Neargal
P 253
1-Methyl-4-Piperidyl benzhydryl ether
4-(Benzhydryloxy)-1-methylpiperidine
Allergen
4-(Diphenylmethoxy)-1-methylpiperidine
N-Methylpiperidyl-(4)-benzhydrylaether salzsauren salze
Diphenylpyralamine

Inchi: InChI=1S/C19H23NO/c1-20-14-12-18(13-15-20)21-19(16-8-4-2-5-9-16)17-10-6-3-7-11-1

InchiKey: OWQUZNMMYNAXSL-UHFFFAOYSA-N

Formula: C19H23NO

SMILES: CN1CCC(OC(c2ccccc2)c2ccccc2)CC1

Mol. weight [g/mol]: 281.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Cheméo Relay (1.0)
logp	3.887		Crippen Method
mcvol	236.040	ml/mol	McGowan Method
rinpol	2101.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook

rinpol	2073.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tf	372.85	K	Cheméo Relay (1.0)

Sources

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C147206&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

tf: Normal melting (fusion) point