Penfluridol

Other names:	4-Piperidinol, 1-[4,4-bis(4-fluorophenyl)butyl]-4-[4-chloro-3-(trifluoromethyl)phenyl]- 4-Piperidinol, 4-(4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-1-(4,4-bis(p-fluorophenyl)butyl)- McN-JR-16,341 R 16341 Semap TLP-607 1-[4,4-Bis(p-fluorophenyl)butyl]-4-(4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-4-p 1-[4,4-Bis(p-flurophenyl)butyl]-4-(4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-4-pi 1-[4,4-Bis(4-fluorophenyl)butyl]-4-[4-chloro-3-(trifluoromethyl)phenyl]-4-piperidinol Penfuridol
Inchi:	InChI=1S/C28H27ClF5NO/c29-26-12-7-21(18-25(26)28(32,33)34)27(36)13-16-35(17-14-
InchiKey:	MDLAAYDRRZXJIF-UHFFFAOYSA-N
Formula:	C28H27ClF5NO
SMILES:	OC1(c2ccc(Cl)c(C(F)(F)F)c2)CCN(CCCC(c2ccc(F)cc2)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	523.97
CAS:	26864-56-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.85		Crippen Method
logp	7.533		Crippen Method
mcvol	360.180	ml/mol	McGowan Method
rinpol	3311.00		NIST Webbook
rinpol	3311.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26864562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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