Diphenidol

Other names:	1-Piperidinebutanol, «alpha»,«alpha»-diphenyl- Benzhydrol, «alpha»-(3-piperidinopropyl)- Difenidol «alpha»,«alpha»-Diphenyl-1-piperidinebutanol Nometic SKF 478 SK&F 478 Vontrol Avomol Cephadol Diphenyl(3-(1-piperidyl)propyl)carbinol
Inchi:	InChI=1S/C21H27NO/c23-21(19-11-4-1-5-12-19,20-13-6-2-7-14-20)15-10-18-22-16-8-3-9
InchiKey:	OGAKLTJNUQRZJU-UHFFFAOYSA-N
Formula:	C21H27NO
SMILES:	OC(CCCN1CCCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	309.45
CAS:	972-02-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	4.189		Crippen Method
mcvol	264.220	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C972021&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