Fenarimol

Other names:	(2-Chlorophenyl)-«alpha»-(4-chlorophenyl)-5-pyrimidinemethanol (2-Chlorophenyl)-Â«alphaÂ»-(4-chlorophenyl)-5-pyrimidinemethanol (2-chlorophenyl)-(4-chlorophenyl)-pyrimidin-5-ylmethanol 2,4'-dichloro-«alpha»(pyrimidin-5-yl)benzhydryl alcohol 2,4'-dichloro-Â«alphaÂ»(pyrimidin-5-yl)benzhydryl alcohol 5-Pyrimidinemethanol, «alpha»-(2-chlorophenyl)-«alpha»-(4-chlorophenyl)- 5-Pyrimidinemethanol, Â«alphaÂ»-(2-chlorophenyl)-Â«alphaÂ»-(4-chlorophenyl)- BLOC EL 222 Rimidin Rubigan «alpha»-(2-Chlorophenyl)-«alpha»-(4-chlorophenyl)-5-pyrimidinemethanol Â«alphaÂ»-(2-Chlorophenyl)-Â«alphaÂ»-(4-chlorophenyl)-5-pyrimidinemethanol
Inchi:	InChI=1S/C17H12Cl2N2O/c18-14-7-5-12(6-8-14)17(22,13-9-20-11-21-10-13)15-3-1-2-4-1
InchiKey:	NHOWDZOIZKMVAI-UHFFFAOYSA-N
Formula:	C17H12Cl2N2O
SMILES:	OC(c1ccc(Cl)cc1)(c1cncnc1)c1ccccc1Cl
Mol. weight [g/mol]:	331.20
CAS:	60168-88-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Aqueous Solubility Prediction Method
log10ws	-4.38		Estimated Solubility Method
logp	4.068		Crippen Method
mcvol	229.420	ml/mol	McGowan Method
rinpol	2602.00		NIST Webbook
rinpol	2561.00		NIST Webbook
rinpol	2602.00		NIST Webbook
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
rinpol	2602.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60168889&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