Triarimol

Other names:	5-Pyrimidinemethanol, «alpha»-(2,4-dichlorophenyl)-«alpha»-phenyl- EL 273 «alpha»-(2,4-Dichlorophenyl)-«alpha»-phenyl-5-pyrimidinemethanol Trimidal Phenyl-(2,4-dichlorophenyl)-(5-pyrimidinyl)carbinol
Inchi:	InChI=1S/C17H12Cl2N2O/c18-14-6-7-15(16(19)8-14)17(22,12-4-2-1-3-5-12)13-9-20-11-
InchiKey:	MYUPFXPCYUISAG-UHFFFAOYSA-N
Formula:	C17H12Cl2N2O
SMILES:	OC(c1ccccc1)(c1cncnc1)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	331.20
CAS:	26766-27-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	4.068		Crippen Method
mcvol	229.420	ml/mol	McGowan Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
ripol	3800.00		NIST Webbook
ripol	3800.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26766278&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
ripol:	Polar retention indices