

Propiconazole

Other names:

1-[[2-(2,4-Dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole
1H-1,2,4-Triazole, 1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-
Aidol SW 900
Banner
Bumper
CGA-64250
CGD 92710F
Desmel
Orbit
Proconazole
Propiconazole II
Propiconizole
Radar
Tilt

Inchi:

InChI=1S/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6

InchiKey:

STJLVHWMYQXCPB-UHFFFAOYSA-N

Formula:

C15H17Cl2N3O2

SMILES:

CCCC1COC(Cn2cncn2)(c2ccc(Cl)cc2Cl)O1

Mol. weight [g/mol]:

342.22

CAS:

75881-82-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Estimated Solubility Method
logp	3.653		Crippen Method
mcvol	234.290	ml/mol	McGowan Method
rinpol	2305.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2357.00		NIST Webbook

Sources

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=C60207901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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