Clotrimazole

Other names:

(2-Chlorophenyl)diphenyl-1-imidazolylmethane
(Chlorotrityl)imidazole
1-((2-chlorophenyl)diphenylmethyl)-1H-imidazole
1-(o-Chloro-«alpha»,«alpha»-diphenylbenzyl)imidazole
1-(o-Chlorophenyldiphenylmethyl)imidazole
1-(o-Chlorotrityl)imidazole
1-(«alpha»-(2-Chlorophenyl)benzhydryl)imidazole
1H-Imidazole, 1-[(2-chlorophenyl)diphenylmethyl]-
BAY 5097
Bay B 5097
Bay B 9057
Bis-phenyl-(2-chlorophenyl)-1-imidazoyl)methane
Bisphenyl-(2-chlorphenyl)-1-imidazolyl-methan
Canesten
Canifug
Chlotrimazole
Clotrimazol
Desamix F
Diphenyl(2-chlorophenyl)(1-imidazolyl)methane
Empecid
FB 5097
Fem Care
Gyne lotrimin
Imidazole, 1-(o-chloro-«alpha»,«alpha»-diphenylbenzyl)-
Lotrimin
Lotrimin AF Cream
Lotrimin AF Solution
Methane, bis-phenyl-(2-chlorophenyl)-1-imidazolyl-
Mono-baycuten
Mycelax
Mycelex
Mycelex 7
Mycelex G
Mycelex OTC
Mycofug
Mycosporin
Mykosporin
NSC 257473
Pedisafe
Rimazole

	Tibatin
	Trimysten
	Veltrim
Inchi:	InChI=1S/C22H17ClN2/c23-21-14-8-7-13-20(21)22(25-16-15-24-17-25,18-9-3-1-4-10-18)
InchiKey:	VNFPBHJOKIVQEB-UHFFFAOYSA-N
Formula:	C22H17ClN2
SMILES:	Clc1ccccc1C(c1ccccc1)(c1ccccc1)n1ccnc1
Mol. weight [g/mol]:	344.84
CAS:	23593-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	5.377		Crippen Method
mcvol	262.300	ml/mol	McGowan Method
tf	416.15	K	Experimental solubility of clotrimazole and some thermodynamic aspects of dissolution in different solvents

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and correlation of antifungal drugs solubility in pure supercritical CO2 using semiempirical models:	https://www.doi.org/10.1016/j.jct.2011.02.020
Experimental solubility of clotrimazole and some thermodynamic aspects of dissolution in different solvents:	https://www.doi.org/10.1016/j.tca.2019.178431
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23593751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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