

AZACONAZOLE

Other names:	1H-1,2,4-Triazole, 1-[[2-(2,4-dichlorophenyl)-1,3-dioxolan-2-yl]methyl]-1-[[2-(2,4-Dichlorophenyl)-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole Azoconazole R-28644
Inchi:	InChI=1S/C12H11Cl2N3O2/c13-10-3-9(4-11(14)5-10)12(18-1-2-19-12)6-17-8-15-7-16-17
InchiKey:	ULXPFHRWKJWAAE-UHFFFAOYSA-N
Formula:	C12H11Cl2N3O2
SMILES:	Clc1cc(Cl)cc(C2(Cn3cncn3)OCCO2)c1
Mol. weight [g/mol]:	300.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Cheméo Relay (1.0)
logp	2.485		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
rinpol	2216.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C60207310&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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<https://www.chemeo.com/cid/13-066-4/AZACONAZOLE.pdf>

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