

Uniconazole

Other names:

1H-1,2,4-Triazole-1-ethanol,
«beta»-[(4-chlorophenyl)methylene]-«alpha»-(1,1-dimethylethyl)-(E)-(.+/-)-
S 3307D

Uniconazole-P

XE 1019

XE 1019D

Inchi:

1H-1,2,4-Triazole-1-ethanol,
«beta»-[(4-chlorophenyl)methylene]-«alpha»-(1,1-dimethylethyl)-(«beta»E)-
InChI=1S/C15H18ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h

InchiKey:

YNWVFADWVLCOPU-MDWZMJQESA-N

Formula:

C15H18ClN3O

SMILES:

CC(C)(C)C(O)C(=Cc1ccc(Cl)cc1)n1cncn1

Mol. weight [g/mol]:

291.78

CAS:

83657-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method
logp	3.337		Crippen Method
mcvol	222.740	ml/mol	McGowan Method
rinpola	2193.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C83657221&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

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

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.cheméo.com/cid/37-261-1/Uniconazole.pdf>

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