Tebuconazole

Other names:
(.+/-.)-Tebuconazole
(.+/-.)-«alpha»-[2-(4-Chlorophenyl)ethyl]-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-e
(RS)-1-(4-chlorophenyl)-4,4-dimethyl-3-(1H-1,2,4-triazol-1-ylmethyl)pentan-3-ol
*
1H-1,2,4-Triazole-1-ethanol, «alpha»-(2-(4-chlorophenyl)ethyl)-«alpha»-(1,1-dimethylethyl)-, (.+/-.)-
1H-1,2,4-Triazole-1-ethanol, «alpha»-[2-(4-chlorophenyl)ethyl]-«alpha»-(1,1-dimethylethyl)-
BAY-HWG 1608
Corail
Elite
Ethyltrianol
Etiltrianol
Fenetrazole
Folicur
HWG 1608
Horizon
Horizont
Lynx
Preventol A 8
Raxil
Tebuconazol
Terbuconazole
Terbutrazole
«alpha»-(2-(4-Chlorophenyl)ethyl)-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanc

Inchi: InChI=1S/C16H22ClN3O/c1-15(2,3)16(21,10-20-12-18-11-19-20)9-8-13-4-6-14(17)7-5-1
InchiKey: PXMNMQRDXWABCY-UHFFFAOYSA-N
Formula: C16H22ClN3O
SMILES: CC(C)(C)C(O)(CCc1ccc(Cl)cc1)Cn1cncn1
Mol. weight [g/mol]: 307.82
CAS: 107534-96-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Cheméo Relay (1.0)
logp	3.342		Crippen Method
mcvol	241.130	ml/mol	McGowan Method
rinpol	2421.00		NIST Webbook

rinpol	2421.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2398.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tf	375.55	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107534963&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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