Hexaconazole

Other names: (Rs)-2-(2,4-dichlorophenyl)-1-(1H-1,2,4-triazol-1-yl)hexan-2-ol
(±)-a-butyl-a-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol
.alpha.-butyl-.alpha.-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol
1H-1,2,4-Triazole-1-ethanol, «alpha»-butyl-«alpha»-(2,4-dichlorophenyl)-
1H-1,2,4-triazole-1-ethanol, .alpha.-butyl-.alpha.-(2,4-dichlorophenyl)-
1H-1,2,4-triazole-1-ethanol, .alpha.-butyl-.alpha.-(2,4-dichlorophenyl)-, (.+-.)-
PP 523
anvil
clortriafol
contaf
contaf 5EC
«alpha»-Butyl-«alpha»-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol (.+/-.)-
«alpha»-butyl-«alpha»-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol
(±)-hexaconazole

Inchi: InChI=1S/C14H17Cl2N3O/c1-2-3-6-14(20,8-19-10-17-9-18-19)12-5-4-11(15)7-13(12)16/h

InchiKey: STMIIPIFODONDC-UHFFFAOYSA-N

Formula: C14H17Cl2N3O

SMILES: CCCCC(O)(Cn1cncn1)c1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 314.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Cheméo Relay (1.0)
logp	3.663		Crippen Method
mcvol	225.190	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tf	342.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hsubt	160.10	kJ/mol	338.00	NIST Webbook
rhos	1331.00	kg/m3	296.00	Thermodynamic properties of diniconazole and hexaconazole

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermodynamic properties of diniconazole and hexaconazole:	https://www.doi.org/10.1016/j.jct.2016.04.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79983714&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point