1H-1,2,4-Triazole-1-ethanol, «alpha»-butyl-«alpha»-(2,4-dichlorophenyl)-, (.+/-.)-

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
hexaconazole
«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/l
InchiKey: STMIIPIFODONDC-UHFFFAOYSA-N
Formula: C14H17Cl2N3O
SMILES: CCCCC(O)(Cn1cncn1)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 314.21
CAS: 79983-71-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	3.663		Crippen Method
mcvol	225.190	ml/mol	McGowan Method
rinpol	2161.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2150.00		NIST Webbook

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
Thermodynamic properties of diniconazole and hexaconazole:	https://www.doi.org/10.1016/j.jct.2016.04.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79983714&Units=SI

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

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