

# 1H-1,2,4-Triazole-1-ethanol, «beta»-[(2,4-dichlorophenyl)methylene]-«alpha»-

Other names:

(E)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)-1-penten-3-ol

1-(2,4-Dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)pent-1-en-3-ol

1H-1,2,4-Triazole-1-ethanol,

«beta»-[(2,4-dichlorophenyl)methylene]-«alpha»-(1,1-dimethylethyl)-, («beta»E)-  
Diniconazole

Diniconazole

Inchi: InChI=1S/C15H17Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)

InchiKey: NSLVZQNHO CYSEE-UHFFFAOYSA-N

Formula: C15H17Cl2N3O

SMILES: CC(C)(C)C(=O)C(Cc1ccc(Cl)cc1Cl)n1cncn1

Mol. weight [g/mol]: 326.22

CAS: 83657-24-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.34		Crippen Method
logp	3.984		Crippen Method
mcvol	234.980	ml/mol	McGowan Method
rinpol	2370.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1323.00	kg/m <sup>3</sup>	296.00	Thermodynamic properties of diniconazole and hexaconazole

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C83657243&Units=SI>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rhos:</b>	Solid Density
<b>rinpola:</b>	Non-polar retention indices

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