

1H-1,2,4-Triazole-1-ethanol, «beta»-((2,4-dichlorophenyl)methyl)-«alpha»-(1,1-

Other names: 1-(2,4-Dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)pentan-3-ol

Diclobutrazol

PP296

Vigil

Diclobutrazole

Dichlobutrazol

Inchi: InChI=1S/C15H19Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)

InchiKey: URDNHJIVMYZFRT-UHFFFAOYSA-N

Formula: C15H19Cl2N3O

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

Mol. weight [g/mol]: 328.24

CAS: 75736-33-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	3.776		Crippen Method
mcvol	239.280	ml/mol	McGowan Method
rinpol	2191.00		NIST Webbook
rinpol	2201.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C75736333&Units=SI>

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

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

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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