

1-[2-(2,4-dichlorophenyl)pentyl]-1H-1,2,4-triazole

Other names:

1-[2-(2,4-Dichlorophenyl)pentyl]-1H-1,2,4-triazole
1-[2-(2,4-Dichlorophenyl)pentyl]-1H-1,2,4-triazole (penconazole)
1H-1,2,4-Triazole, 1-[2-(2,4-dichlorophenyl)pentyl]-
Award
CGA 71818
Topas 100
Topaz
Topaze

Inchi: InChI=1S/C13H15Cl2N3/c1-2-3-10(7-18-9-16-8-17-18)12-5-4-11(14)6-13(12)15/h4-6,8-1

InchiKey: WKBPZYKAUNRMKP-UHFFFAOYSA-N

Formula: C13H15Cl2N3

SMILES: CCCC(Cn1cncn1)c1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 284.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Cheméo Relay (1.0)
logp	4.169		Crippen Method
mcvol	205.230	ml/mol	McGowan Method

Sources

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

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):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C66246886>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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