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