

Penconazole

Other names:	1H-1,2,4-Triazole, 1-[2-(2,4-dichlorophenyl)pentyl]- 1-[2-(2,4-Dichlorophenyl)pentyl]-1H-1,2,4-triazole Award CGA 71818 Topas 100 Topaz Topaze 1-[2-(2,4-Dichlorophenyl)pentyl]-1H-1,2,4-triazole (penconazole)
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]:	284.18
CAS:	87501-25-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	4.169		Crippen Method
mcvol	205.230	ml/mol	McGowan Method
rinpol	2054.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2048.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.58	kJ/mol	332.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66246886&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
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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