Fenbuconazole

Other names:	1H-1,2,4-Triazole-1-propanenitrile, «alpha»-[2-(4-chlorophenyl)ethyl]-«alpha»-phenyl- 1H-1,2,4-Triazole-1-propanenitrile, Â«alphaÂ»-[2-(4-chlorophenyl)ethyl]-Â«alphaÂ»-phenyl-
Inchi:	InChI=1S/C19H17ClN4/c20-18-8-6-16(7-9-18)10-11-19(12-21,13-24-15-22-14-23-24)17-
InchiKey:	RQDJADAKIFFEKQ-UHFFFAOYSA-N
Formula:	C19H17ClN4
SMILES:	N#CC(CCc1ccc(Cl)cc1)(Cn1cncn1)c1ccccc1
Mol. weight [g/mol]:	336.82
CAS:	114369-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.23		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.026		Crippen Method
mcvol	255.150	ml/mol	McGowan Method
rinpol	2782.00		NIST Webbook
rinpol	2776.00		NIST Webbook
rinpol	2782.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114369436&Units=SI

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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