TEBUFENPYRAD

Other names:	1H-Pyrazole-5-carboxamide, 4-chloro-N-[[4-(1,1-dimethylethyl)phenyl]methyl]-3-ethyl-1-methyl-
Inchi:	InChI=1S/C18H24ClN3O/c1-6-14-15(19)16(22(5)21-14)17(23)20-11-12-7-9-13(10-8-12)1
InchiKey:	ZZYSLNWGKKDOML-UHFFFAOYSA-N
Formula:	C18H24ClN3O
SMILES:	CCc1nn(C)c(C(=O)NCc2ccc(C(C)(C)C)cc2)c1Cl
Mol. weight [g/mol]:	333.86
CAS:	119168-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	3.863		Crippen Method
mcvol	265.010	ml/mol	McGowan Method
rinpol	2497.00		NIST Webbook
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
rinpol	2497.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119168773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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