Tolfenpyrad

Other names: 1H-Pyrazole-5-carboxamide, 4-chloro-3-ethyl-1-methyl-N-[[4-(4-methylphenoxy)phenyl]methyl]-
Inchi: InChI=1S/C21H22ClN3O2/c1-4-18-19(22)20(25(3)24-18)21(26)23-13-15-7-11-17(12-8-15
InchiKey: WPALTCMYPARVNV-UHFFFAOYSA-N
Formula: C21H22ClN3O2
SMILES: CCc1nn(C)c(C(=O)NCc2ccc(Oc3ccc(C)cc3)cc2)c1Cl
Mol. weight [g/mol]: 383.87
CAS: 129558-76-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.58		Crippen Method
logp	4.667		Crippen Method
mcvol	289.390	ml/mol	McGowan Method
rinpol	3106.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C129558765&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices