Pyriminobac-methyl (Z)

Inchi: InChI=1S/C17H19N3O6/c1-10(20-25-5)11-7-6-8-12(15(11)16(21)24-4)26-17-18-13(22-2)
InchiKey: USSIUIGPBLPCDF-JMIUGGIZSA-N
Formula: C17H19N3O6
SMILES: CON=C(C)c1cccc(Oc2nc(OC)cc(OC)n2)c1C(=O)OC
Mol. weight [g/mol]: 361.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.443		Crippen Method
mcvol	259.430	ml/mol	McGowan Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R566739&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.