maltoxazine

Inchi: InChI=1S/C10H13NO2/c12-8-4-3-7-6-13-9-2-1-5-11(9)10(7)8/h9H,1-6H2
InchiKey: MTHASAHNRVFFOM-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: O=C1CCC2=C1N1CCCC1OC2
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	1.055		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
rinpol	1630.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225097&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