Quinoline, 5-(phenylazo)-

Other names: Orotic acid, triTBDMS
Inchi: InChI=1S/C15H11N3/c1-2-6-12(7-3-1)17-18-15-10-4-9-14-13(15)8-5-11-16-14/h1-11H
InchiKey: RQIJYXYCHYDCDC-UHFFFAOYSA-N
Formula: C15H11N3
SMILES: c1ccc(N=Nc2cccc3ncccc23)cc1
Mol. weight [g/mol]: 233.27
CAS: 25117-46-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.650		Crippen Method
mcvol	180.870	ml/mol	McGowan Method
rinpol	2393.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117468&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