[1,3]Dioxolo[4,5-j]phenanthridine

Inchi: InChI=1S/C14H9NO2/c1-2-4-12-10(3-1)11-6-14-13(16-8-17-14)5-9(11)7-15-12/h1-7H,8H
InchiKey: RFILRSDHWIIIMN-UHFFFAOYSA-N
Formula: C14H9NO2
SMILES: c1ccc2c(c1)ncc1cc3c(cc12)OCO3
Mol. weight [g/mol]: 223.23
CAS: 224-11-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	3.117		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
rinpol	2273.90		NIST Webbook
rinpol	2273.90		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=C224113&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