3-ethylfuro[2,3-h]quinoline

Inchi: InChI=1S/C13H11NO/c1-2-9-7-10-3-4-12-11(5-6-15-12)13(10)14-8-9/h3-8H,2H2,1H3
InchiKey: UWQCOLOVGFGGOC-UHFFFAOYSA-N
Formula: C13H11NO
SMILES: CCc1cnc2c(ccc3occc32)c1
Mol. weight [g/mol]: 197.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.38		Crippen Method
logp	3.543		Crippen Method
mcvol	151.500	ml/mol	McGowan Method
rinpol	2145.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2145.00		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=R261068&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