

4-(5-Ethylquinuclidine-2-carbonyl)-1,2-dihydro-2-oxoquinoline

Inchi: InChI=1S/C19H22N2O2/c1-2-12-11-21-8-7-13(12)9-17(21)19(23)15-10-18(22)20-16-6-4
InchiKey: CEPOUTOVISPBIE-UHFFFAOYSA-N
Formula: C₁₉H₂₂N₂O₂
SMILES: CCC1CN2CCC1CC2C(=O)c1cc(=O)[nH]c2ccccc12
Mol. weight [g/mol]: 310.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	2.349		Crippen Method
mcvol	241.030	ml/mol	McGowan Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U242754&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

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