4-(5-ETHYLQUINUCLIDINE-2-CARBONYL)-1,2-DIH

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]: 310.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Cheméo Relay (1.0)
logp	2.349		Crippen Method
mcvol	241.030	ml/mol	McGowan Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		NIST Webbook
tf	516.74	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U242754&Units=SI
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
tf: Normal melting (fusion) point