

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:	CCC1CN2CCCC1CC2C(=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

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