Phenanthro[3,2-b]furan-7,11-dione, 1,2,3,4-tetrahydro-4,4,8-trimethyl-

Other names: Isotanshinone II
«alpha»-Isotanshinone

Inchi: InChI=1S/C19H18O3/c1-10-9-22-18-14(10)16(20)12-6-7-13-11(15(12)17(18)21)5-4-8-19

InchiKey: QHGPIJMPUOVBOL-UHFFFAOYSA-N

Formula: C19H18O3

SMILES: Cc1coc2c1C(=O)c1ccc3c(c1C2=O)CCCC3(C)C

Mol. weight [g/mol]: 294.34

CAS: 20958-15-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.85		Crippen Method
logp	3.977		Crippen Method
mcvol	222.640	ml/mol	McGowan Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		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=C20958150&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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