Phenanthro[3,2-b]furan-7,11-dione, 4,8-dimethyl-

Other names: Isotanshinone I
Isotanshinone «alpha»
Inchi: InChI=1S/C18H12O3/c1-9-4-3-5-12-11(9)6-7-13-15(12)17(20)18-14(16(13)19)10(2)8-21-
InchiKey: XYKZSUXWBGUGQV-UHFFFAOYSA-N
Formula: C18H12O3
SMILES: Cc1coc2c1C(=O)c1ccc3c(C)cccc3c1C2=O
Mol. weight [g/mol]: 276.29
CAS: 20958-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.12		Crippen Method
logp	3.825		Crippen Method
mcvol	199.950	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=C20958172&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