Phenanthro[1,2-b]furan-10,11-dione, 1,6-dimethyl-

Other names: Tanshinon I
Tanshinone I
Tanshinone A
1,6-Dimethylphenanthro[1,2-b]furan-10,11-dione

Inchi: InChI=1S/C18H12O3/c1-9-4-3-5-12-11(9)6-7-13-15(12)17(20)16(19)14-10(2)8-21-18(13)

InchiKey: AIGAZQPHXLWMOJ-UHFFFAOYSA-N

Formula: C18H12O3

SMILES: Cc1coc2c1C(=O)C(=O)c1c-2ccc2c(C)cccc12

Mol. weight [g/mol]: 276.29

CAS: 568-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.94		Crippen Method
logp	4.096		Crippen Method
mcvol	199.950	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.09	kJ/mol	495.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C568730&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume