Phenanthro[1,2-b]furan-10,11-dione, 6,7,8,9-tetrahydro-1,6,6-trimethyl-

Other names: 6,7,8,9-Tetrahydro-1,6,6-trimethylphenanthro[1,2-b]furan-10,11-dione
Tanshinon II
Tanshinone 2-A
Tanshinone II
Tanshinone IIA

Inchi: InChI=1S/C19H18O3/c1-10-9-22-18-12-6-7-13-11(5-4-8-19(13,2)3)15(12)17(21)16(20)14

InchiKey: HYXITZLLTYIPOF-UHFFFAOYSA-N

Formula: C19H18O3

SMILES: Cc1coc2c1C(=O)C(=O)c1c-2ccc2c1CCCC2(C)C

Mol. weight [g/mol]: 294.34

CAS: 568-72-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.67		Crippen Method
logp	4.248		Crippen Method
mcvol	222.640	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.17	kJ/mol	486.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C568729&Units=SI

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

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

Solubility of 1,6,6-Trimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione in Four Organic Solvents from (283.2 to 323.3) K: https://www.doi.org/10.1021/je800238y

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