Tanshinone II-b

Other names:	Tanshinone II-b Tanshinon IIB Phenanthro[1,2-b]furan-10,11-dione, 6,7,8,9-tetrahydro-6-(hydroxymethyl)-1,6-dimethyl-, (6S)- 6-(Hydroxymethyl)-1,6-dimethyl-6,7,8,9-tetrahydrophenanthro[1,2-b]furan-10,11-dione, (S)- 6,7,8,9-Tetrahydro-6-(hydroxymethyl)1,6-dimethylphenanthro-[1,2-b]-furan-10,11-dione
Inchi:	InChI=1S/C19H18O4/c1-10-8-23-18-12-5-6-13-11(4-3-7-19(13,2)9-20)15(12)17(22)16(21
InchiKey:	XDUXBBDRILEIEZ-UHFFFAOYSA-N
Formula:	C19H18O4
SMILES:	Cc1coc2c1C(=O)C(=O)c1c-2ccc2c1CCCC2(C)CO
Mol. weight [g/mol]:	310.35

Physical Properties

Property code	Value	Unit	Source
logp	3.220		Crippen Method
mcvol	228.510	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.74	kJ/mol	479.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17397932&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume