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

Latest version available from:

https://www.chemeo.com/cid/91-892-1/Phenanthro-1-2-b-furan-10-11-dione-6-7-8-9-tetrahydro-1-6-6-trimethyl.pdf

Generated by Cheméo on 2024-10-12 08:34:36.606079294 +0000 UTC m=+3302939.243048542.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.