2,3-dihydro-5-hydroxy-6,8,8-trimethyl-2-phenyl-4 H-1-benzopyran-4,7(8 H)-dione, isomer 1, enol form (champanone C)

InchI: InChI=1S/C18H20O4/c1-11-17(21)16-14(19(2,3)18(11)22)9-13(10-15(16)20)12-7-5-4-6-8

InchiKey: XWOZBPADMFCFKZ-UHFFFAOYSA-N

Formula: C18H20O4

SMILES: CC1=C(O)C2=C(CC(c3ccccc3)CC2=O)C(C)(C)C1=O

Mol. weight [g/mol]: 296.36

Physical Properties

Property code	Value	Unit	Source
gf	-71.48	kJ/mol	Joback Method
hf	-420.71	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	87.93	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.871		Crippen Method
mcvol	233.500	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2407.00		NIST Webbook
tb	937.66	K	Joback Method
tc	1185.29	K	Joback Method
tf	624.87	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.02	J/mol×K	937.66	Joback Method
cpg	788.45	J/mol×K	978.93	Joback Method
cpg	805.31	J/mol×K	1020.20	Joback Method
cpg	821.73	J/mol×K	1061.48	Joback Method
cpg	837.85	J/mol×K	1102.75	Joback Method
cpg	853.79	J/mol×K	1144.02	Joback Method
cpg	869.69	J/mol×K	1185.29	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume