2,2,4,4-Tetramethyl-6-(3-phenylpropanoyl)cyclohe

Other names:	1,3,5-Cyclohexanetrione, 2,2,4,4-tetramethyl-6-(1-oxo-3-phenylpropyl)- Champanone E Grandiflorone 2,2,4,4-tetramethyl-6-(3'-phenylpropionyl)cyclohexane-1,3,5-trione, isomer 1 (champanone E)
Inchi:	InChI=1S/C19H22O4/c1-18(2)15(21)14(16(22)19(3,4)17(18)23)13(20)11-10-12-8-6-5-7-9
InchiKey:	HDCYLHJYUHYIQL-UHFFFAOYSA-N
Formula:	C19H22O4
SMILES:	CC1(C)C(=O)C(C(=O)CCc2ccccc2)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]:	314.38
CAS:	50861-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-277.13	kJ/mol	Joback Method
hf	-680.52	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.578		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	928.82	K	Joback Method
tc	1189.26	K	Joback Method
tf	631.60	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.08	J/mol×K	928.82	Joback Method
cpg	865.95	J/mol×K	972.23	Joback Method
cpg	888.67	J/mol×K	1015.63	Joback Method

cpg	911.47	J/mol×K	1059.04	Joback Method
cpg	934.56	J/mol×K	1102.44	Joback Method
cpg	958.16	J/mol×K	1145.85	Joback Method
cpg	982.48	J/mol×K	1189.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50861535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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