2,2,4-trimethyl-6-(1-oxo-3-phenylprop-2-enyl)cyclo enol form (champanone B)

Inchi: InChI=1S/C19H20O4/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: APGSUBPMFNRCHM-ZHACJKMWSA-N

Formula: C19H20O4

SMILES: CC1(C)C(=O)C(C(=O)C=Cc2ccccc2)C(=O)C(C)(C)C1=O

Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
gf	-196.91	kJ/mol	Joback Method
hf	-563.30	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.658		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2498.00		NIST Webbook
tb	932.98	K	Joback Method
tc	1201.79	K	Joback Method
tf	626.52	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.31	J/mol×K	932.98	Joback Method
cpg	838.43	J/mol×K	977.78	Joback Method
cpg	861.64	J/mol×K	1022.58	Joback Method
cpg	885.22	J/mol×K	1067.39	Joback Method
cpg	909.42	J/mol×K	1112.19	Joback Method
cpg	934.51	J/mol×K	1156.99	Joback Method
cpg	960.76	J/mol×K	1201.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435026&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