2,2,4,4-tetramethyl-6-(1-oxo-3-phenylprop-2-enyl)-enol form (champanone A)

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: PEHSOPDEJGYVAH-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	-192.73	kJ/mol	Joback Method
hf	-522.65	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.285		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	971.13	K	Joback Method
tc	1217.78	K	Joback Method
tf	649.16	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.49	J/mol×K	971.13	Joback Method
cpg	831.83	J/mol×K	1012.24	Joback Method
cpg	853.88	J/mol×K	1053.35	Joback Method
cpg	876.90	J/mol×K	1094.46	Joback Method
cpg	901.14	J/mol×K	1135.57	Joback Method
cpg	926.84	J/mol×K	1176.67	Joback Method
cpg	954.24	J/mol×K	1217.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434974&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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