2,2,4-trimethyl-5-cinnamoyl-1,3-cyclopentanedion

Inchi: InChI=1S/C17H18O3/c1-11-14(16(20)17(2,3)15(11)19)13(18)10-9-12-7-5-4-6-8-12/h4-11
InchiKey: CPBSLMYWDXZCCV-MDZDMXLPSA-N
Formula: C17H18O3
SMILES: CC1C(=O)C(C)(C)C(=O)C1C(=O)C=Cc1ccccc1
Mol. weight [g/mol]: 270.32

Physical Properties

Property code	Value	Unit	Source
gf	-73.57	kJ/mol	Joback Method
hf	-393.40	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.699		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	814.89	K	Joback Method
tc	1070.46	K	Joback Method
tf	515.38	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.94	J/mol×K	814.89	Joback Method
cpg	680.95	J/mol×K	857.49	Joback Method
cpg	699.02	J/mol×K	900.08	Joback Method
cpg	716.28	J/mol×K	942.68	Joback Method
cpg	732.88	J/mol×K	985.27	Joback Method
cpg	748.96	J/mol×K	1027.87	Joback Method
cpg	764.68	J/mol×K	1070.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435006&Units=SI

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