2,2,4-trimethyl-5-cinnamoylcyclopent-4-ene-1,3-di

Inchi: InChI=1S/C17H16O3/c1-11-14(16(20)17(2,3)15(11)19)13(18)10-9-12-7-5-4-6-8-12/h4-10
InchiKey: YXVCHJRCRWVPHK-MDZDMXLPSA-N
Formula: C17H16O3
SMILES: CC1=C(C(=O)C=Cc2ccccc2)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
gf	-47.45	kJ/mol	Joback Method
hf	-317.88	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	71.63	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.763		Crippen Method
mcvol	211.880	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook
tb	833.35	K	Joback Method
tc	1091.90	K	Joback Method
tf	549.66	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.39	J/mol×K	833.35	Joback Method
cpg	641.60	J/mol×K	876.44	Joback Method
cpg	658.14	J/mol×K	919.53	Joback Method
cpg	674.18	J/mol×K	962.62	Joback Method
cpg	689.85	J/mol×K	1005.71	Joback Method
cpg	705.33	J/mol×K	1048.80	Joback Method
cpg	720.76	J/mol×K	1091.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435011&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