2,5-Dimethyl-3,4-diphenylcyclopentadienone

Inchi: InChI=1S/C19H16O/c1-13-17(15-9-5-3-6-10-15)18(14(2)19(13)20)16-11-7-4-8-12-16/h3-
InchiKey: SOXYIWTUKPMWCG-UHFFFAOYSA-N
Formula: C19H16O
SMILES: CC1=C(c2ccccc2)C(c2ccccc2)=C(C)C1=O
Mol. weight [g/mol]: 260.33
CAS: 26307-17-5

Physical Properties

Property code	Value	Unit	Source
gf	276.99	kJ/mol	Joback Method
hf	50.37	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	70.48	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.517		Crippen Method
mcvol	213.160	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
tb	793.49	K	Joback Method
tc	1057.72	K	Joback Method
tf	491.69	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.87	J/mol×K	793.49	Joback Method
cpg	614.57	J/mol×K	837.53	Joback Method
cpg	629.74	J/mol×K	881.57	Joback Method
cpg	643.46	J/mol×K	925.60	Joback Method
cpg	655.79	J/mol×K	969.64	Joback Method
cpg	666.79	J/mol×K	1013.68	Joback Method
cpg	676.54	J/mol×K	1057.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26307175&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume