Cyclohexanone, 2,2-dimethyl-6,6-diphenyl-

Inchi: InChI=1S/C20H22O/c1-19(2)14-9-15-20(18(19)21,16-10-5-3-6-11-16)17-12-7-4-8-13-17/
InchiKey: LKGJEIWVWSCBGA-UHFFFAOYSA-N
Formula: C20H22O
SMILES: CC1(C)CCCC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 278.39
CAS: 50592-53-5

Physical Properties

Property code	Value	Unit	Source
gf	225.51	kJ/mol	Joback Method
hf	-56.31	kJ/mol	Joback Method
hfus	15.46	kJ/mol	Joback Method
hvap	66.73	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.752		Crippen Method
mcvol	235.850	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
tb	793.54	K	Joback Method
tc	1072.16	K	Joback Method
tf	487.16	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.02	J/mol×K	793.54	Joback Method
cpg	737.14	J/mol×K	839.98	Joback Method
cpg	760.81	J/mol×K	886.41	Joback Method
cpg	784.48	J/mol×K	932.85	Joback Method
cpg	808.60	J/mol×K	979.29	Joback Method
cpg	833.61	J/mol×K	1025.72	Joback Method
cpg	859.96	J/mol×K	1072.16	Joback Method

Sources

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=C50592535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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