Cyclohexanone, 2-(3-chloro-2-butenyl)-2-methyl-6,6-diphenyl-

Inchi: InChI=1S/C23H25ClO/c1-18(24)14-17-22(2)15-9-16-23(21(22)25,19-10-5-3-6-11-19)20-1

InchiKey: TWBAHMRTJVSXOP-NBVRZTHBSA-N

Formula: C23H25ClO

SMILES: CC(Cl)=CCC1(C)CCCC(c2ccccc2)(c2ccccc2)C1=O

Mol. weight [g/mol]: 352.90

CAS: 50592-54-6

Physical Properties

Property code	Value	Unit	Source
gf	310.51	kJ/mol	Joback Method
hf	-26.54	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.265		Crippen Method
mcvol	286.060	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
tb	903.65	K	Joback Method
tc	1177.97	K	Joback Method
tf	531.85	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.59	J/mol×K	903.65	Joback Method
cpg	922.46	J/mol×K	949.37	Joback Method
cpg	948.92	J/mol×K	995.09	Joback Method
cpg	976.43	J/mol×K	1040.81	Joback Method
cpg	1005.47	J/mol×K	1086.53	Joback Method
cpg	1036.54	J/mol×K	1132.25	Joback Method
cpg	1070.10	J/mol×K	1177.97	Joback Method

Sources

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=C50592546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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