2-Cyclopropen-1-one, 2,3-diphenyl-

Other names:	Cyclopropenone, diphenyl-
	Cyclopropenone, 2,3-diphenyl-
	Diphenylcyclopropenone
	2,3-Diphenylcyclopropenone
	2,3-Diphenyl-2-cyclopropen-1-one
	Diphencyprone
	DPC
	2,3-diphenylcycloprop-2-en-1-one
Inchi:	InChI=1S/C15H10O/c16-15-13(11-7-3-1-4-8-11)14(15)12-9-5-2-6-10-12/h1-10H
InchiKey:	HCIBTBXNLVOFER-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	O=c1c(-c2ccccc2)c1-c1ccccc1
Mol. weight [g/mol]:	206.24
CAS:	886-38-4

Physical Properties

Property code	Value	Unit	Source
chl	-7562.00 ± 20.00	kJ/mol	NIST Webbook
chs	-7742.90	kJ/mol	NIST Webbook
chs	-7529.80 ± 1.80	kJ/mol	NIST Webbook
hf	317.70 ± 8.20	kJ/mol	NIST Webbook
hf	552.30	kJ/mol	NIST Webbook
hf	360.00 ± 20.00	kJ/mol	NIST Webbook
hfs	198.00 ± 2.00	kJ/mol	NIST Webbook
hsub	119.70 ± 8.00	kJ/mol	NIST Webbook
ie	10.56	eV	NIST Webbook
ie	8.47	eV	NIST Webbook
log10ws	-4.93		Crippen Method
logp	3.256		Crippen Method
mcvol	161.100	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hsubt	120.00 ± 8.00	kJ/mol	365.50	NIST Webbook
hsubt	141.00 ± 4.20	kJ/mol	323.00	NIST Webbook
hsubt	141.00 ± 4.00	kJ/mol	333.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C886384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume