2-Cyclohexen-1-one, 3-phenyl-

Other names:	1-Phenylcyclohexen-3-one
	3-Phenyl-2-cyclohexenone
	3-phenylcyclohex-2-en-1-one
Inchi:	InChI=1S/C12H12O/c13-12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-3,5-6,9H,4,7-8H2
InchiKey:	DIELDZAPFMXAHA-UHFFFAOYSA-N
Formula:	C12H12O
SMILES:	O=C1C=C(c2ccccc2)CCC1
Mol. weight [g/mol]:	172.22
CAS:	10345-87-6

Physical Properties

Property code	Value	Unit	Source
gf	92.47	kJ/mol	Joback Method
hf	-71.21	kJ/mol	Joback Method
hfus	11.98	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.823		Crippen Method
mcvol	142.590	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	596.82	K	Joback Method
tc	856.41	K	Joback Method
tf	344.54	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.49	J/mol×K	596.82	Joback Method
cpg	362.45	J/mol×K	640.09	Joback Method
cpg	379.08	J/mol×K	683.35	Joback Method
cpg	394.41	J/mol×K	726.62	Joback Method
cpg	408.47	J/mol×K	769.88	Joback Method
cpg	421.28	J/mol×K	813.15	Joback Method

cpg	432.89	J/mol×K	856.41	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=C10345876&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