Ethanone, 1,2-diphenyl-

Other names:	Acetophenone, 2-phenyl-
	Benzoin, deoxy-
	Benzyl phenyl ketone
	Deoxybenzoin
	Desoxybenzoin
	Phenyl benzyl ketone
	1,2-Diphenylethanone
	2-Phenylacetophenone
	1,2-Diphenylethan-1-one
Inchi:	InChI=1S/C14H12O/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey:	OTKCEEWUXHVZQI-UHFFFAOYSA-N
Formula:	C14H12O
SMILES:	O=C(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	196.24
CAS:	451-40-1

Physical Properties

Property code	Value	Unit	Source
chs	-7153.00 ± 3.00	kJ/mol	NIST Webbook
gf	162.90	kJ/mol	Joback Method
hf	28.19	kJ/mol	Joback Method
hfs	-71.09	kJ/mol	NIST Webbook
hfus	21.70	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-3.75		Crippen Method
logp	3.112		Crippen Method
mcvol	162.170	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1537.10		NIST Webbook
tb	593.20	K	NIST Webbook
tc	873.70	K	Joback Method
tf	330.00 ± 4.00	K	NIST Webbook
tf	329.00 ± 3.00	K	NIST Webbook
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.79	J/mol×K	873.70	Joback Method
cpg	457.69	J/mol×K	832.57	Joback Method
cpg	446.61	J/mol×K	791.45	Joback Method
cpg	434.48	J/mol×K	750.32	Joback Method
cpg	421.20	J/mol×K	709.20	Joback Method
cpg	406.71	J/mol×K	668.07	Joback Method
cpg	390.90	J/mol×K	626.95	Joback Method
dvisc	0.0021880	Pa×s	350.31	Joback Method
dvisc	0.0001896	Pa×s	626.95	Joback Method
dvisc	0.0002425	Pa×s	580.84	Joback Method
dvisc	0.0003235	Pa×s	534.74	Joback Method
dvisc	0.0004556	Pa×s	488.63	Joback Method
dvisc	0.0006893	Pa×s	442.52	Joback Method
dvisc	0.0011483	Pa×s	396.42	Joback Method
hvapt	68.10	kJ/mol	495.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C451401&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization 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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume