2-Propanone, 1,3-diphenyl-

Other names:	«alpha»,«alpha»'-Diphenylacetone
	Benzyl ketone
	Dibenzyl ketone
	1,3-Diphenyl-2-propanone
	1,3-Diphenylacetone
	1,3-Diphenylpropanone
	1,3-Diphenyl-propan-2-one
	NSC 220312
Inchi:	InChI=1S/C15H14O/c16-15(11-13-7-3-1-4-8-13)12-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	YFKBXYGUSOXJGS-UHFFFAOYSA-N
Formula:	C15H14O
SMILES:	O=C(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	210.27
CAS:	102-04-5

Physical Properties

Property code	Value	Unit	Source
chs	-7819.50 ± 2.50	kJ/mol	NIST Webbook
gf	171.32	kJ/mol	Joback Method
hf	7.55	kJ/mol	Joback Method
hfs	-84.00 ± 2.60	kJ/mol	NIST Webbook
hfus	24.29	kJ/mol	Joback Method
hsub	89.10	kJ/mol	NIST Webbook
hvap	60.28	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.041		Crippen Method
mcvol	176.260	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	173.60		NIST Webbook
tb	604.20	K	NIST Webbook
tc	891.24	K	Joback Method
tf	308.00 ± 1.00	K	NIST Webbook
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.79	J/mol×K	891.24	Joback Method
cpg	440.98	J/mol×K	649.83	Joback Method
cpg	457.27	J/mol×K	690.06	Joback Method
cpg	472.25	J/mol×K	730.30	Joback Method
cpg	486.02	J/mol×K	770.53	Joback Method
cpg	498.64	J/mol×K	810.77	Joback Method
cpg	510.20	J/mol×K	851.00	Joback Method
dvisc	0.0001726	Pa×s	649.83	Joback Method
dvisc	0.0020973	Pa×s	361.58	Joback Method
dvisc	0.0010836	Pa×s	409.62	Joback Method
dvisc	0.0006431	Pa×s	457.66	Joback Method
dvisc	0.0004215	Pa×s	505.70	Joback Method
dvisc	0.0002972	Pa×s	553.75	Joback Method
dvisc	0.0002216	Pa×s	601.79	Joback Method
hfust	20.20	kJ/mol	307.20	NIST Webbook
hfust	20.20	kJ/mol	307.20	NIST Webbook
hvapt	65.70	kJ/mol	501.00	NIST Webbook
sfust	65.78	J/mol×K	307.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102045&Units=SI
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

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume