1-Butanone, 1-phenyl-

Other names:	Butyrophenone
	n-Butyrophenone
	Phenyl propyl ketone
	Propyl phenyl ketone
	1-Phenyl-1-butanone
Inchi:	InChI=1S/C10H12O/c1-2-6-10(11)9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3
InchiKey:	FFSAXUULYPJSKH-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CCCC(=O)c1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	495-40-9

Physical Properties

Property code	Value	Unit	Source
chl	-5461.30 ± 1.70	kJ/mol	NIST Webbook
gf	16.81	kJ/mol	Joback Method
hf	-125.78	kJ/mol	Joback Method
hfl	-188.80 ± 1.90	kJ/mol	NIST Webbook
hfus	17.30	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
ie	9.40 ± 0.20	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.669		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1275.60		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1270.20		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1265.30		NIST Webbook
rinpol	1267.90		NIST Webbook
rinpol	1252.20		NIST Webbook

rinpol	1261.00		NIST Webbook
rinpol	1285.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1792.00		NIST Webbook
tb	501.70	K	NIST Webbook
tc	723.65	K	Joback Method
tf	278.81	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.61	J/mol×K	508.75	Joback Method
cpg	290.55	J/mol×K	544.57	Joback Method
cpg	303.65	J/mol×K	580.38	Joback Method
cpg	315.93	J/mol×K	616.20	Joback Method
cpg	327.44	J/mol×K	652.02	Joback Method
cpg	338.20	J/mol×K	687.83	Joback Method
cpg	348.26	J/mol×K	723.65	Joback Method
dvisc	0.0031046	Pa×s	278.81	Joback Method
dvisc	0.0015984	Pa×s	317.13	Joback Method
dvisc	0.0009496	Pa×s	355.46	Joback Method
dvisc	0.0006244	Pa×s	393.78	Joback Method
dvisc	0.0004422	Pa×s	432.10	Joback Method
dvisc	0.0003313	Pa×s	470.43	Joback Method
dvisc	0.0002592	Pa×s	508.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.00 ± 1.00	K	2.70	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=C495409&Units=SI

Legend

chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume