1-Pentanone, 1-phenyl-

Other names:	Valerophenone
	Butyl phenyl ketone
	1-Phenyl-1-pentanone
	Pentanophenone
Inchi:	InChI=1S/C11H14O/c1-2-3-9-11(12)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3
InchiKey:	XKGLSKVNOSHTAD-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	162.23
CAS:	1009-14-9

Physical Properties

Property code	Value	Unit	Source
gf	25.23	kJ/mol	Joback Method
hf	-146.42	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
log10ws	-3.39		Crippen Method
logp	3.060		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1365.70		NIST Webbook
rinpol	1378.70		NIST Webbook
rinpol	1366.20		NIST Webbook
rinpol	1372.60		NIST Webbook
rinpol	1359.50		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1355.60		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1376.00		NIST Webbook

rinpol	1376.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1373.20		NIST Webbook
rinpol	1372.60		NIST Webbook
rinpol	1373.20		NIST Webbook
tb	531.63	K	Joback Method
tc	743.09	K	Joback Method
tf	290.08	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.62	J/mol×K	531.63	Joback Method
cpg	336.43	J/mol×K	566.87	Joback Method
cpg	350.36	J/mol×K	602.12	Joback Method
cpg	363.44	J/mol×K	637.36	Joback Method
cpg	375.71	J/mol×K	672.61	Joback Method
cpg	387.21	J/mol×K	707.85	Joback Method
cpg	397.96	J/mol×K	743.09	Joback Method
dvisc	0.0031127	Pa×s	290.08	Joback Method
dvisc	0.0015721	Pa×s	330.34	Joback Method
dvisc	0.0009211	Pa×s	370.60	Joback Method
dvisc	0.0005992	Pa×s	410.86	Joback Method
dvisc	0.0004210	Pa×s	451.11	Joback Method
dvisc	0.0003133	Pa×s	491.37	Joback Method
dvisc	0.0002439	Pa×s	531.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	0.70	NIST Webbook

Sources

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=C1009149&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume