1-Octanone, 1-phenyl-

Other names:	Octanophenone
	n-Octanophenone
	Caprylophenone
	Heptyl phenyl ketone
	Ketone, heptyl phenyl
	1-phenyloctan-1-one
Inchi:	InChI=1S/C14H20O/c1-2-3-4-5-9-12-14(15)13-10-7-6-8-11-13/h6-8,10-11H,2-5,9,12H2,1
InchiKey:	UDEVCZRUNOLVLU-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	CCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	204.31
CAS:	1674-37-9

Physical Properties

Property code	Value	Unit	Source
gf	50.49	kJ/mol	Joback Method
hf	-208.34	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.230		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
tb	560.70	K	NIST Webbook
tc	802.16	K	Joback Method
tf	323.89	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.92	J/mol×K	600.27	Joback Method
cpg	541.39	J/mol×K	768.51	Joback Method
cpg	528.26	J/mol×K	734.86	Joback Method

cpg	514.28	J/mol×K	701.21	Joback Method
cpg	499.43	J/mol×K	667.57	Joback Method
cpg	483.65	J/mol×K	633.92	Joback Method
cpg	553.72	J/mol×K	802.16	Joback Method
dvisc	0.0001908	Pa×s	600.27	Joback Method
dvisc	0.0002485	Pa×s	554.21	Joback Method
dvisc	0.0003395	Pa×s	508.14	Joback Method
dvisc	0.0004937	Pa×s	462.08	Joback Method
dvisc	0.0007799	Pa×s	416.02	Joback Method
dvisc	0.0013807	Pa×s	369.95	Joback Method
dvisc	0.0028754	Pa×s	323.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	2.00	NIST Webbook
tbrp	440.00 ± 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=C1674379&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume