1-Hexanone, 1-phenyl-

Other names:	Hexanophenone
	Caprophenone
	Hexaphenone
	Pentyl phenyl ketone
	1-Phenyl-1-hexanone
	n-Amylphenyl ketone
	n-Hexanophenone
Inchi:	InChI=1S/C12H16O/c1-2-3-5-10-12(13)11-8-6-4-7-9-11/h4,6-9H,2-3,5,10H2,1H3
InchiKey:	MAHPVQDVMLWUAG-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	176.25
CAS:	942-92-7

Physical Properties

Property code	Value	Unit	Source
gf	33.65	kJ/mol	Joback Method
hf	-167.06	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.450		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1470.80		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1478.70		NIST Webbook
rinpol	1459.90		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1482.40		NIST Webbook
rinpol	1467.70		NIST Webbook
rinpol	1475.70		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1437.00		NIST Webbook

rinpol	1478.70		NIST Webbook
rinpol	1475.70		NIST Webbook
tb	538.20	K	NIST Webbook
tc	762.63	K	Joback Method
tf	301.35	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.41	J/mol×K	554.51	Joback Method
cpg	383.97	J/mol×K	589.20	Joback Method
cpg	398.61	J/mol×K	623.88	Joback Method
cpg	412.38	J/mol×K	658.57	Joback Method
cpg	425.31	J/mol×K	693.25	Joback Method
cpg	437.43	J/mol×K	727.94	Joback Method
cpg	448.79	J/mol×K	762.63	Joback Method
dvisc	0.0030718	Pa×s	301.35	Joback Method
dvisc	0.0015239	Pa×s	343.54	Joback Method
dvisc	0.0008813	Pa×s	385.74	Joback Method
dvisc	0.0005678	Pa×s	427.93	Joback Method
dvisc	0.0003958	Pa×s	470.12	Joback Method
dvisc	0.0002929	Pa×s	512.32	Joback Method
dvisc	0.0002268	Pa×s	554.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	2.00	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=C942927&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
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