1-PHENYL-PENTAN-2-ONE

Other names:	1-Phenyl-2-pentanone
	1-phenylpentan-2-one
	Benzyl propyl ketone
Inchi:	InChI=1S/C11H14O/c1-2-6-11(12)9-10-7-4-3-5-8-10/h3-5,7-8H,2,6,9H2,1H3
InchiKey:	NFKAWBGFIMBUMB-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CCCC(=O)Cc1ccccc1
Mol. weight [g/mol]:	162.23

Physical Properties

Property code	Value	Unit	Source
af	0.4705		Cheméo Relay (1.0)
gf	25.23	kJ/mol	Joback Method
hf	-142.78	kJ/mol	Cheméo Relay (1.0)
hfus	19.89	kJ/mol	Joback Method
hvap	52.46	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-2.29		Cheméo Relay (1.0)
logp	2.598		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	516.51	K	Cheméo Relay (1.0)
tc	720.92	K	Cheméo Relay (1.0)
tf	281.01	K	Cheméo Relay (1.0)
vc	0.517	m3/kmol	Cheméo Relay (1.0)

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	410.85	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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6683927&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume