

2-Pentanone, 1-phenyl-

Other names:	Benzyl propyl ketone 1-Phenyl-2-pentanone 1-phenylpentan-2-one
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
CAS:	6683-92-7

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
log10ws	-2.81		Crippen Method
logp	2.598		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
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/molxK	531.63	Joback Method
cpg	336.43	J/molxK	566.87	Joback Method
cpg	350.36	J/molxK	602.12	Joback Method
cpg	363.44	J/molxK	637.36	Joback Method
cpg	375.71	J/molxK	672.61	Joback Method
cpg	387.21	J/molxK	707.85	Joback Method

cpg	397.96	J/mol×K	743.09	Joback Method
dvisc	0.0031127	Paxs	290.08	Joback Method
dvisc	0.0015721	Paxs	330.34	Joback Method
dvisc	0.0009211	Paxs	370.60	Joback Method
dvisc	0.0005992	Paxs	410.86	Joback Method
dvisc	0.0004210	Paxs	451.11	Joback Method
dvisc	0.0003133	Paxs	491.37	Joback Method
dvisc	0.0002439	Paxs	531.63	Joback Method

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=C6683927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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