2-Pentanone, 5-phenyl-

Other names: Methyl 3-phenylpropyl ketone
5-Phenyl-2-pentanone
5-phenylpentan-2-one
Inchi: InChI=1S/C11H14O/c1-10(12)6-5-9-11-7-3-2-4-8-11/h2-4,7-8H,5-6,9H2,1H3
InchiKey: DGMYRPFYNFQCHM-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 162.23
CAS: 2235-83-8

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	9.00 ± 0.10	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	2.598		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
ripol	1942.00		NIST Webbook
ripol	1942.00		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

Sources

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=C2235838&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume