2,4-Pentanedione, 3-phenyl-

Other names:	3-Phenyl-2,4-pentanedione
	3-Phenylacetylacetone
Inchi:	InChI=1S/C11H12O2/c1-8(12)11(9(2)13)10-6-4-3-5-7-10/h3-7,11H,1-2H3
InchiKey:	YIWTXSVNRCWBAC-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	CC(=O)C(C(C)=O)c1ccccc1
Mol. weight [g/mol]:	176.21
CAS:	5910-25-8

Physical Properties

Property code	Value	Unit	Source
gf	-106.13	kJ/mol	Joback Method
hf	-264.28	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.948		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1633.00		NIST Webbook
tb	585.06	K	Joback Method
tc	809.43	K	Joback Method
tf	325.01	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.88	J/mol×K	585.06	Joback Method
cpg	353.65	J/mol×K	622.46	Joback Method
cpg	366.48	J/mol×K	659.85	Joback Method
cpg	378.41	J/mol×K	697.25	Joback Method
cpg	389.48	J/mol×K	734.64	Joback Method
cpg	399.74	J/mol×K	772.04	Joback Method

cpg	409.22	J/mol×K	809.43	Joback Method
dvisc	0.0033356	Pa×s	325.01	Joback Method
dvisc	0.0016707	Pa×s	368.35	Joback Method
dvisc	0.0009679	Pa×s	411.69	Joback Method
dvisc	0.0006222	Pa×s	455.03	Joback Method
dvisc	0.0004319	Pa×s	498.38	Joback Method
dvisc	0.0003179	Pa×s	541.72	Joback Method
dvisc	0.0002448	Pa×s	585.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5910258&Units=SI
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

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

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