1,4-Pentanedione, 1-phenyl-

Other names:	1-Phenyl-1,4-pentanedione
Inchi:	InChI=1S/C11H12O2/c1-9(12)7-8-11(13)10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey:	RBLXWIPBPPVLPU-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	CC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	176.21
CAS:	583-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-103.69	kJ/mol	Joback Method
hf	-259.00	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.239		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	585.50	K	Joback Method
tc	805.11	K	Joback Method
tf	340.01	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.46	J/mol×K	585.50	Joback Method
cpg	352.88	J/mol×K	622.10	Joback Method
cpg	365.41	J/mol×K	658.70	Joback Method
cpg	377.09	J/mol×K	695.31	Joback Method
cpg	387.96	J/mol×K	731.91	Joback Method
cpg	398.06	J/mol×K	768.51	Joback Method
cpg	407.41	J/mol×K	805.11	Joback Method
dvisc	0.0026331	Pa×s	340.01	Joback Method

dvisc	0.0014576	Pa×s	380.93	Joback Method
dvisc	0.0009050	Pa×s	421.84	Joback Method
dvisc	0.0006113	Pa×s	462.75	Joback Method
dvisc	0.0004401	Pa×s	503.67	Joback Method
dvisc	0.0003329	Pa×s	544.59	Joback Method
dvisc	0.0002618	Pa×s	585.50	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=C583051&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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