

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:	RBLXWIPBPPVLPV-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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.46	J/molxK	585.50	Joback Method
cpg	398.06	J/molxK	768.51	Joback Method
cpg	387.96	J/molxK	731.91	Joback Method
cpg	377.09	J/molxK	695.31	Joback Method
cpg	365.41	J/molxK	658.70	Joback Method
cpg	352.88	J/molxK	622.10	Joback Method
cpg	407.41	J/molxK	805.11	Joback Method
dvisc	0.0002618	Paxs	585.50	Joback Method

dvisc	0.0003329	Paxs	544.59	Joback Method
dvisc	0.0004401	Paxs	503.67	Joback Method
dvisc	0.0006113	Paxs	462.75	Joback Method
dvisc	0.0009050	Paxs	421.84	Joback Method
dvisc	0.0014576	Paxs	380.93	Joback Method
dvisc	0.0026331	Paxs	340.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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