1,5-Pentanedione, 3-methyl-1,5-diphenyl-

Inchi: InChI=1S/C18H18O2/c1-14(12-17(19)15-8-4-2-5-9-15)13-18(20)16-10-6-3-7-11-16/h2-11
InchiKey: NXXCHGCIGOMMIZ-UHFFFAOYSA-N
Formula: C18H18O2
SMILES: CC(CC(=O)c1ccccc1)CC(=O)c1ccccc1
Mol. weight [g/mol]: 266.33
CAS: 1226-91-1

Physical Properties

Property code	Value	Unit	Source
gf	65.22	kJ/mol	Joback Method
hf	-172.23	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.168		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	771.90	K	Joback Method
tc	1009.01	K	Joback Method
tf	430.32	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.39	J/mol×K	771.90	Joback Method
cpg	681.75	J/mol×K	969.49	Joback Method
cpg	670.90	J/mol×K	929.98	Joback Method
cpg	659.02	J/mol×K	890.46	Joback Method
cpg	646.03	J/mol×K	850.94	Joback Method
cpg	631.85	J/mol×K	811.42	Joback Method
cpg	691.68	J/mol×K	1009.01	Joback Method
dvisc	0.0001149	Pa×s	771.90	Joback Method
dvisc	0.0001502	Pa×s	714.97	Joback Method

dvisc	0.0002058	Pa×s	658.04	Joback Method
dvisc	0.0002993	Pa×s	601.11	Joback Method
dvisc	0.0004708	Pa×s	544.18	Joback Method
dvisc	0.0008232	Pa×s	487.25	Joback Method
dvisc	0.0016687	Pa×s	430.32	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=C1226911&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