1,3-Propanedione,2,2-dimethyl-1,3-diphenyl-

Other names: 2,2-Dimethyl-1,3-diphenyl-1,3-propanedione
Inchi: InChI=1S/C17H16O2/c1-17(2,15(18)13-9-5-3-6-10-13)16(19)14-11-7-4-8-12-14/h3-12H,1
InchiKey: ZCQWHDYGRXASIN-UHFFFAOYSA-N
Formula: C17H16O2
SMILES: CC(C)(C(=O)c1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]: 252.31
CAS: 41169-42-0

Physical Properties

Property code	Value	Unit	Source
gf	62.08	kJ/mol	Joback Method
hf	-155.06	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	70.18	kJ/mol	Joback Method
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-4.62		Crippen Method
logp	3.778		Crippen Method
mcvol	206.010	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
tb	746.23	K	Joback Method
tc	996.72	K	Joback Method
tf	436.47	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.88	J/mol×K	746.23	Joback Method
cpg	579.29	J/mol×K	787.98	Joback Method
cpg	593.31	J/mol×K	829.73	Joback Method
cpg	606.07	J/mol×K	871.48	Joback Method
cpg	617.70	J/mol×K	913.22	Joback Method
cpg	628.34	J/mol×K	954.97	Joback Method
cpg	638.10	J/mol×K	996.72	Joback Method

dvisc	0.0015226	Pa×s	436.47	Joback Method
dvisc	0.0007894	Pa×s	488.10	Joback Method
dvisc	0.0004640	Pa×s	539.72	Joback Method
dvisc	0.0002993	Pa×s	591.35	Joback Method
dvisc	0.0002071	Pa×s	642.98	Joback Method
dvisc	0.0001514	Pa×s	694.60	Joback Method
dvisc	0.0001156	Pa×s	746.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41169420&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
ie:	Ionization energy
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