1,2-Propanedione, 1-phenyl-

Other names:	Acetylbenzoyl
	Benzoyl methyl ketone
	Benzoylacetyl
	Methylphenylglyoxal
	Phenylmethyldiketone
	Pyruvophenone
	1-Phenyl-1,2-propanedione
	3-Phenyl-2,3-propanedione
	Methyl phenyl diketone
	1-Phenyl-1,2-propandione
	1-phenylpropane-1,2-dione
Inchi:	InChI=1S/C9H8O2/c1-7(10)9(11)8-5-3-2-4-6-8/h2-6H,1H3
InchiKey:	BVQVLAIMHVDZEL-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	CC(=O)C(=O)c1ccccc1
Mol. weight [g/mol]:	148.16
CAS:	579-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-120.53	kJ/mol	Joback Method
hf	-217.72	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	51.40	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.458		Crippen Method
mcvol	117.050	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1186.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1166.10		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1166.10		NIST Webbook
rinpol	1175.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1818.00		NIST Webbook

ripol	1818.00		NIST Webbook
tb	539.74	K	Joback Method
tc	767.58	K	Joback Method
tf	317.47	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.60	J/mol×K	539.74	Joback Method
cpg	260.27	J/mol×K	577.71	Joback Method
cpg	271.12	J/mol×K	615.69	Joback Method
cpg	281.20	J/mol×K	653.66	Joback Method
cpg	290.54	J/mol×K	691.63	Joback Method
cpg	299.17	J/mol×K	729.61	Joback Method
cpg	307.13	J/mol×K	767.58	Joback Method
dvisc	0.0026925	Pa×s	317.47	Joback Method
dvisc	0.0015470	Pa×s	354.52	Joback Method
dvisc	0.0009871	Pa×s	391.56	Joback Method
dvisc	0.0006807	Pa×s	428.61	Joback Method
dvisc	0.0004980	Pa×s	465.65	Joback Method
dvisc	0.0003815	Pa×s	502.69	Joback Method
dvisc	0.0003032	Pa×s	539.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	1.90	NIST Webbook

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=C579077&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume