1,3-Butanedione, 1-phenyl-

Other names:	«alpha»-Acetylacetophenone
	Acetoacetophenone
	Acetylbenzoylmethane
	Benzoylacetone
	1-Benzoyl-2-propanone
	1-Phenyl-1,3-butanedione
	2-Acetylacetophenone
	2-Propanone, benzoyl-
	1-Benzoylacetone
	Benzoyl-aceton
	NSC 4015
	1-phenylbutane-1,3-dione
Inchi:	InChI=1S/C10H10O2/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	CVBUKMMMRLOKQR-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	CC(=O)CC(=O)c1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	93-91-4

Physical Properties

Property code	Value	Unit	Source
chl	-5024.50 ± 5.40	kJ/mol	NIST Webbook
chs	-5029.10 ± 2.50	kJ/mol	NIST Webbook
gf	-112.11	kJ/mol	Joback Method
hf	-284.40	kJ/mol	NIST Webbook
hf	-251.30 ± 2.90	kJ/mol	NIST Webbook
hf	-244.10 ± 2.90	kJ/mol	NIST Webbook
hfl	-340.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-335.10 ± 2.80	kJ/mol	NIST Webbook
hfus	18.89	kJ/mol	Joback Method
hsub	83.80	kJ/mol	NIST Webbook
hsub	91.00 ± 0.60	kJ/mol	NIST Webbook
hsub	91.01 ± 0.63	kJ/mol	NIST Webbook
hvap	55.60	kJ/mol	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.848		Crippen Method

mcvol	131.140	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	533.15 ± 3.00	K	NIST Webbook
tc	786.27	K	Joback Method
tf	331.00 ± 3.00	K	NIST Webbook
tf	333.15 ± 1.00	K	NIST Webbook
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.17	J/mol×K	562.62	Joback Method
cpg	305.78	J/mol×K	599.90	Joback Method
cpg	317.53	J/mol×K	637.17	Joback Method
cpg	328.47	J/mol×K	674.45	Joback Method
cpg	338.63	J/mol×K	711.72	Joback Method
cpg	348.04	J/mol×K	749.00	Joback Method
cpg	356.75	J/mol×K	786.27	Joback Method
dvisc	0.0015118	Pa×s	367.72	Joback Method
dvisc	0.0026820	Pa×s	328.74	Joback Method
dvisc	0.0009511	Pa×s	406.70	Joback Method
dvisc	0.0006489	Pa×s	445.68	Joback Method
dvisc	0.0004708	Pa×s	484.66	Joback Method
dvisc	0.0003583	Pa×s	523.64	Joback Method
dvisc	0.0002832	Pa×s	562.62	Joback Method
hsubt	83.70	kJ/mol	289.00	NIST Webbook
hsubt	83.76 ± 0.42	kJ/mol	331.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93914&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

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume