1,4-Butanedione, 1,4-diphenyl-

Other names:	1,2-Dibenzoylethane
	1,4-Diphenyl-1,4-butanedione
	2,2''-Biacetophenone
	Biphenacyl
	Dibenzoylethane
	Ethane, 1,2-dibenzoyl-
Inchi:	InChI=1S/C16H14O2/c17-15(13-7-3-1-4-8-13)11-12-16(18)14-9-5-2-6-10-14/h1-10H,11-1
InchiKey:	OSWWFLDIIGGSJV-UHFFFAOYSA-N
Formula:	C16H14O2
SMILES:	O=C(CCC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	238.28
CAS:	495-71-6

Physical Properties

Property code	Value	Unit	Source
chs	-8041.40 ± 1.50	kJ/mol	NIST Webbook
chs	-8036.20	kJ/mol	NIST Webbook
gf	50.82	kJ/mol	Joback Method
hf	-125.67	kJ/mol	Joback Method
hfs	-261.00	kJ/mol	NIST Webbook
hfs	-255.60 ± 1.50	kJ/mol	NIST Webbook
hfus	28.48	kJ/mol	Joback Method
hvap	69.25	kJ/mol	Joback Method
ie	9.20 ± 0.05	eV	NIST Webbook
log10ws	-4.44		Crippen Method
logp	3.532		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
ss	324.79	J/mol×K	NIST Webbook
tb	726.58	K	Joback Method
tc	968.53	K	Joback Method
tf	418.60 ± 0.20	K	NIST Webbook
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.30	J/mol×K	726.58	Joback Method
cpg	522.95	J/mol×K	766.90	Joback Method
cpg	536.35	J/mol×K	807.23	Joback Method
cpg	548.58	J/mol×K	847.55	Joback Method
cpg	559.74	J/mol×K	887.88	Joback Method
cpg	569.89	J/mol×K	928.20	Joback Method
cpg	579.14	J/mol×K	968.53	Joback Method
cps	302.10	J/mol×K	303.00	NIST Webbook
cps	291.20	J/mol×K	296.00	NIST Webbook
dvisc	0.0001581	Pa×s	726.58	Joback Method
dvisc	0.0009090	Pa×s	473.41	Joback Method
dvisc	0.0016581	Pa×s	422.78	Joback Method
dvisc	0.0003753	Pa×s	574.68	Joback Method
dvisc	0.0002685	Pa×s	625.31	Joback Method
dvisc	0.0002020	Pa×s	675.95	Joback Method
dvisc	0.0005597	Pa×s	524.05	Joback Method
hfust	38.98	kJ/mol	418.60	NIST Webbook
hfust	38.99	kJ/mol	418.60	NIST Webbook
hfust	0.22	kJ/mol	187.00	NIST Webbook
hfust	38.99	kJ/mol	418.60	NIST Webbook
sfust	93.10	J/mol×K	418.60	NIST Webbook
sfust	1.17	J/mol×K	187.00	NIST Webbook
sfust	93.30	J/mol×K	418.60	NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C495716&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume