Ethanedione, diphenyl-

Other names:	1,2-Diphenylethane-1,2-dione
	1,2-Diphenylethanedione
	1,2-Ethanedione, 1,2-diphenyl-
	Benzil
	Bibenzoyl
	Dibenzoyl
	Diphenyl-«alpha»,«beta»-diketone
	Diphenyl-Â«alphaÂ»,Â«betaÂ»-diketone
	Diphenylethanedione
	Diphenylglyoxal
	Glyoxal, diphenyl-
	NSC 220315
	Wy 20910
Inchi:	InChI=1S/C14H10O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10H
InchiKey:	WURBFLDFSFBTLW-UHFFFAOYSA-N
Formula:	C14H10O2
SMILES:	O=C(C(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	210.23
CAS:	134-81-6

Physical Properties

Property code	Value	Unit	Source
chs	-6760.00 ± 3.00	kJ/mol	NIST Webbook
chs	-6784.00 ± 3.00	kJ/mol	NIST Webbook
chs	-6828.70	kJ/mol	NIST Webbook
chs	-6784.80	kJ/mol	NIST Webbook
gf	33.98	kJ/mol	Joback Method
hf	-84.39	kJ/mol	Joback Method
hfs	-179.00	kJ/mol	NIST Webbook
hfs	138.00	kJ/mol	NIST Webbook
hfs	-154.00	kJ/mol	NIST Webbook
hfus	23.30	kJ/mol	Joback Method
hsub	87.40	kJ/mol	NIST Webbook
hvap	64.80	kJ/mol	Joback Method
ie	8.86 ± 0.15	eV	NIST Webbook
ie	8.78 ± 0.05	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook

ie	9.10	eV	NIST Webbook
ie	8.68 ± 0.05	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-3.08		Aqueous Solubility Prediction Method
logp	2.752		Crippen Method
mcvol	163.740	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1768.00		NIST Webbook
sg	480.18	J/mol×K	NIST Webbook
ss	292.08	J/mol×K	NIST Webbook
tb	620.00 ± 1.00	K	NIST Webbook
tc	933.59	K	Joback Method
tf	368.50	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	368.00 ± 2.00	K	NIST Webbook
tf	368.01	K	Aqueous Solubility Prediction Method
tf	368.25 ± 1.00	K	NIST Webbook
tf	368.00	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tf	369.30 ± 0.60	K	NIST Webbook
tf	368.15 ± 1.00	K	NIST Webbook
tf	368.25 ± 0.20	K	NIST Webbook
tf	368.00	K	NIST Webbook
tf	368.15 ± 2.00	K	NIST Webbook
tf	367.00 ± 1.00	K	NIST Webbook
tf	368.05 ± 0.20	K	NIST Webbook
tt	368.02 ± 0.01	K	NIST Webbook
tt	368.00 ± 0.00	K	NIST Webbook
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.72	J/mol×K	891.46	Joback Method

cpg	405.45	J/mol×K	680.82	Joback Method
cpg	443.16	J/mol×K	807.21	Joback Method
cpg	453.44	J/mol×K	849.33	Joback Method
cpg	471.08	J/mol×K	933.59	Joback Method
cpg	431.79	J/mol×K	765.08	Joback Method
cpg	419.25	J/mol×K	722.95	Joback Method
cps	245.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0010540	Pa×s	447.00	Joback Method
dvisc	0.0002487	Pa×s	634.06	Joback Method
dvisc	0.0003274	Pa×s	587.29	Joback Method
dvisc	0.0001962	Pa×s	680.82	Joback Method
dvisc	0.0018672	Pa×s	400.24	Joback Method
dvisc	0.0004519	Pa×s	540.53	Joback Method
dvisc	0.0006630	Pa×s	493.77	Joback Method
hfust	0.04	kJ/mol	84.00	NIST Webbook
hfust	22.69	kJ/mol	368.05	NIST Webbook
hfust	23.56	kJ/mol	368.00	NIST Webbook
hfust	23.80	kJ/mol	369.20	NIST Webbook
hfust	22.88	kJ/mol	368.10	NIST Webbook
hfust	23.56	kJ/mol	368.00	NIST Webbook
hsubt	82.80 ± 0.80	kJ/mol	311.00	NIST Webbook
hsubt	98.40 ± 1.10	kJ/mol	368.50	NIST Webbook
hsubt	98.40 ± 1.10	kJ/mol	329.50	NIST Webbook
hvapt	69.20	kJ/mol	510.50	NIST Webbook
sfust	64.02	J/mol×K	368.00	NIST Webbook
sfust	0.50	J/mol×K	84.00	NIST Webbook
sfust	61.65	J/mol×K	368.05	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.00	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.56292e+01
Coeff. B	-6.38708e+03
Coeff. C	-3.99290e+01
Temperature range (K), min.	456.25
Temperature range (K), max.	658.97

Sources

Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C134816&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibrium of Rebaudioside A in Pure and Binary Mixed Solvents at T = (288.15 to 328.15) K:	https://www.doi.org/10.1021/acs.jced.8b00780
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Water and Organic Solvents at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00065
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:	https://www.doi.org/10.1016/j.tca.2012.03.028
Solubilities of Three Flavonoids in Different Natural Deep Eutectic Solvents at T = (288.15 to 328.15) K:	https://www.doi.org/10.1021/acs.jced.6b00552

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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