Dibenzofuran

Other names:	2,2'-Biphenylene oxide
	2,2'-Biphenylylene oxide
	Dibenzo[b,d]furan
	Dibenzofurane
	Diphenylene oxide
	[1,1'-Biphenyl]-2,2'-diyl oxide
	dibenzo[bd]furan
Inchi:	InChI=1S/C12H8O/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H
InchiKey:	TXCDCPKCNAJMEE-UHFFFAOYSA-N
Formula:	C12H8O
SMILES:	c1ccc2c(c1)oc1ccccc12
Mol. weight [g/mol]:	168.19
CAS:	132-64-9

Physical Properties

Property code	Value	Unit	Source
chs	-5859.70 ± 4.20	kJ/mol	NIST Webbook
chs	-5836.30 ± 4.70	kJ/mol	NIST Webbook
hf	47.30 ± 4.80	kJ/mol	NIST Webbook
hfs	-29.20 ± 4.80	kJ/mol	NIST Webbook
hsub	82.00 ± 0.20	kJ/mol	NIST Webbook
hsub	76.46 ± 0.16	kJ/mol	NIST Webbook
hsub	84.40 ± 0.70	kJ/mol	NIST Webbook
hsub	76.50 ± 0.20	kJ/mol	NIST Webbook
hsub	88.70	kJ/mol	NIST Webbook
hsub	76.50	kJ/mol	NIST Webbook
ie	7.90 ± 0.05	eV	NIST Webbook
ie	8.22	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
log10ws	-4.51		Aqueous Solubility Prediction Method
log10ws	-4.60		Estimated Solubility Method
logp	3.586		Crippen Method
mcvol	127.430	ml/mol	McGowan Method
pc	3640.00 ± 100.00	kPa	NIST Webbook

rhoc	339.75 ± 5.05	kg/m3	NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1549.20		NIST Webbook
rinpol	1499.40		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1520.90		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1519.60		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	260.30		NIST Webbook
rinpol	260.40		NIST Webbook
rinpol	252.13		NIST Webbook
rinpol	259.74		NIST Webbook
rinpol	1520.90		NIST Webbook
rinpol	257.02		NIST Webbook
rinpol	259.70		NIST Webbook
rinpol	259.50		NIST Webbook
rinpol	258.80		NIST Webbook
rinpol	259.57		NIST Webbook
rinpol	257.12		NIST Webbook
rinpol	259.07		NIST Webbook
rinpol	259.75		NIST Webbook
rinpol	254.58		NIST Webbook
rinpol	252.50		NIST Webbook

rinpol	258.77		NIST Webbook
rinpol	257.17		NIST Webbook
rinpol	260.80		NIST Webbook
rinpol	259.63		NIST Webbook
rinpol	259.07		NIST Webbook
rinpol	259.63		NIST Webbook
rinpol	251.74		NIST Webbook
rinpol	258.70		NIST Webbook
rinpol	259.74		NIST Webbook
rinpol	263.31		NIST Webbook
rinpol	258.53		NIST Webbook
rinpol	261.30		NIST Webbook
rinpol	258.80		NIST Webbook
rinpol	259.10		NIST Webbook
rinpol	256.05		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	259.80		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1499.40		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1517.50		NIST Webbook
rinpol	1494.90		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	258.72		NIST Webbook
rinpol	257.17		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2308.00		NIST Webbook
ripol	256.99		NIST Webbook
ripol	2308.00		NIST Webbook
ss	196.18	J/mol×K	NIST Webbook
tb	558.20	K	NIST Webbook
tb	560.20	K	NIST Webbook
tb	560.15 ± 0.60	K	NIST Webbook
tc	824.00 ± 4.00	K	NIST Webbook
tf	355.66	K	Solid-liquid equilibrium of some polycyclic aromatic hydrocarbons in wash oil
tf	356.32	K	Aqueous Solubility Prediction Method
tt	355.31	K	KDB
tt	355.31 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	199.01	J/mol×K	298.15	NIST Webbook
hfust	18.60	kJ/mol	354.70	NIST Webbook
hfust	19.41	kJ/mol	355.10	NIST Webbook
hfust	20.50	kJ/mol	355.80	NIST Webbook
hfust	17.60	kJ/mol	355.20	NIST Webbook
hfust	18.60	kJ/mol	355.70	NIST Webbook
hfust	18.60	kJ/mol	355.70	NIST Webbook
hsubt	82.10 ± 1.50	kJ/mol	306.50	NIST Webbook
hsubt	85.60	kJ/mol	323.50	NIST Webbook
hsubt	79.10	kJ/mol	323.00	NIST Webbook
hsubt	76.70	kJ/mol	322.50	NIST Webbook
hvapt	66.20	kJ/mol	398.00	NIST Webbook
hvapt	55.10	kJ/mol	481.00	NIST Webbook
hvapt	66.20	kJ/mol	410.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45387e+01
Coeff. B	-5.25976e+03
Coeff. C	-2.99520e+01
Temperature range (K), min.	355.65
Temperature range (K), max.	599.98

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C132649&Units=SI

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1041

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solid-liquid phase equilibrium of 9-fluorenone and several polynuclear aromatic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.01.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solubilities of Selected PCDDs and PCDFs in Water and Various Chloride Solutions:	https://www.doi.org/10.1021/je700185m
Cosolvent Effect of Methanol and Acetic Acid on Dibenzofuran Solubility in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je800574v
Solid-Liquid Phase Equilibrium and Solubility of Dibenzo[b,d]furan and 9H-Fluoren-9-one in Organic Solvents:	https://www.doi.org/10.1021/je201282d
Solid-liquid equilibrium of some polycyclic aromatic hydrocarbons in wash oil:	https://www.doi.org/10.1016/j.fluid.2012.01.031
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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