Benzene, 1,1'-oxybis-

Other names:	1,1'-OXYBIS-BENZENE
	1,1'-Oxybisbenzene
	Benzene, phenoxy-
	Biphenyl oxide
	Chemcryl JK-EB
	Ether, diphenyl-
	Geranium crystals
	NSC 19311
	Oxybisbenzene
	Oxydiphenyl
	PHENOXY BENZENE
	Phenyl oxide
	diphenyl ether
	diphenyl oxide
	phenoxybenzene
	phenyl ether
Inchi:	InChI=1S/C12H10O/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10H
InchiKey:	USIUVYZYUHIAEV-UHFFFAOYSA-N
Formula:	C12H10O
SMILES:	c1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	170.21
CAS:	101-84-8

Physical Properties

Property code	Value	Unit	Source
af	0.4400		KDB
chl	-6113.70 ± 3.80	kJ/mol	NIST Webbook
chs	-6119.24 ± 0.88	kJ/mol	NIST Webbook
dm	1.10	debye	KDB
gf	169.98	kJ/mol	Joback Method
hf	49.99	kJ/mol	KDB
hfs	-32.11 ± 0.93	kJ/mol	NIST Webbook
hfus	17.12	kJ/mol	Standard enthalpy of formation of diphenyl oxide
hvap	64.90 ± 2.10	kJ/mol	NIST Webbook
hvap	66.10 ± 0.40	kJ/mol	NIST Webbook
hvap	66.90 ± 0.30	kJ/mol	NIST Webbook

hvap	65.00	kJ/mol	NIST Webbook
hvap	67.10	kJ/mol	NIST Webbook
ie	8.09 ± 0.03	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.82 ± 0.05	eV	NIST Webbook
log10ws	-3.96		Estimated Solubility Method
log10ws	-3.93		Aqueous Solubility Prediction Method
logp	3.479		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	3141.07 ± 202.65	kPa	NIST Webbook
pc	3140.00	kPa	KDB
rinpol	1380.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1370.90		NIST Webbook
rinpol	1366.40		NIST Webbook
rinpol	1381.70		NIST Webbook
rinpol	1393.70		NIST Webbook
rinpol	1380.10		NIST Webbook
rinpol	1384.60		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1356.90		NIST Webbook
rinpol	1372.60		NIST Webbook
rinpol	1371.80		NIST Webbook
rinpol	1376.20		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1389.90		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	241.70		NIST Webbook
rinpol	241.16		NIST Webbook
rinpol	241.70		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1396.00		NIST Webbook

rinpol	1366.40		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1376.30		NIST Webbook
rinpol	1366.80		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2017.00		NIST Webbook
ss	233.91	J/mol×K	NIST Webbook
tb	531.46 ± 0.07	K	NIST Webbook
tb	531.20	K	KDB
tb	532.20	K	NIST Webbook
tb	531.10	K	NIST Webbook
tb	523.65 ± 1.50	K	NIST Webbook
tb	532.50 ± 0.50	K	NIST Webbook
tc	766.80	K	KDB
tc	767.20 ± 1.00	K	NIST Webbook
tc	788.15 ± 2.00	K	NIST Webbook
tc	766.80 ± 1.00	K	NIST Webbook
tf	300.00 ± 0.02	K	NIST Webbook
tf	300.05 ± 0.05	K	NIST Webbook
tf	299.90 ± 0.02	K	NIST Webbook
tf	300.02	K	KDB
tf	300.04 ± 0.01	K	NIST Webbook
tf	300.58 ± 0.20	K	NIST Webbook
tf	300.60	K	Aqueous Solubility Prediction Method
tf	300.20 ± 0.20	K	NIST Webbook
tf	299.90 ± 0.30	K	NIST Webbook
tf	299.90 ± 0.40	K	NIST Webbook
tf	300.15 ± 1.00	K	NIST Webbook
tt	300.03 ± 0.01	K	NIST Webbook
tt	300.03 ± 0.01	K	NIST Webbook
tt	300.01 ± 0.00	K	NIST Webbook
vc	0.510	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.80	J/mol×K	549.74	Joback Method
cpg	318.62	J/mol×K	590.77	Joback Method
cpg	333.25	J/mol×K	631.80	Joback Method
cpg	346.73	J/mol×K	672.82	Joback Method
cpg	359.14	J/mol×K	713.85	Joback Method
cpg	370.51	J/mol×K	754.88	Joback Method
cpg	380.90	J/mol×K	795.91	Joback Method
cps	215.90	J/mol×K	298.50	NIST Webbook
cps	216.56	J/mol×K	298.15	NIST Webbook
cps	216.56	J/mol×K	298.15	NIST Webbook
dvisc	0.0006136	Pa×s	383.29	Joback Method
dvisc	0.0010297	Pa×s	341.68	Joback Method
dvisc	0.0002874	Pa×s	466.52	Joback Method
dvisc	0.0019947	Pa×s	300.07	Joback Method
dvisc	0.0004047	Pa×s	424.90	Joback Method
dvisc	0.0001694	Pa×s	549.74	Joback Method
dvisc	0.0002159	Pa×s	508.13	Joback Method
hfust	17.21	kJ/mol	300.00	NIST Webbook
hfust	17.21	kJ/mol	300.03	NIST Webbook
hfust	17.22	kJ/mol	300.02	NIST Webbook
hfust	17.21	kJ/mol	300.00	NIST Webbook
hfust	16.51	kJ/mol	300.40	NIST Webbook
hfust	17.21	kJ/mol	300.03	NIST Webbook
hvapt	48.20	kJ/mol	510.50	NIST Webbook
hvapt	64.20	kJ/mol	323.00	NIST Webbook
hvapt	53.00	kJ/mol	510.50	NIST Webbook
pvap	0.04	kPa	331.50	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	6.46e-03	kPa	308.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	7.44e-03	kPa	310.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	5.31e-03	kPa	305.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	4.26e-03	kPa	303.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	2.93e-03	kPa	299.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	9.68e-03	kPa	313.40	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.01	kPa	315.30	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	319.40	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	323.40	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.03	kPa	327.40	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	328.90	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.05	kPa	335.50	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.06	kPa	339.60	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.09	kPa	343.70	Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

rhol	1039.60	kg/m3	333.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1065.50	kg/m3	303.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1005.20	kg/m3	373.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1013.70	kg/m3	363.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1022.30	kg/m3	353.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1030.90	kg/m3	343.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	
rhol	1048.20	kg/m3	323.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures	

rhol	1056.90	kg/m3	313.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures
rhol	1061.20	kg/m3	308.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures
rhol	1066.00	kg/m3	303.00	KDB
sfust	57.38	J/mol×K	300.03	NIST Webbook
sfust	57.38	J/mol×K	300.02	NIST Webbook
sfust	57.38	J/mol×K	300.03	NIST Webbook
tcondl	0.15	W/m×K	343.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids
tcondl	0.14	W/m×K	333.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids
tcondl	0.14	W/m×K	323.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids
tcondl	0.13	W/m×K	313.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids
tcondl	0.13	W/m×K	303.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44628e+01
Coeff. B	-4.38113e+03
Coeff. C	-8.71630e+01
Temperature range (K), min.	396.23
Temperature range (K), max.	565.91

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1031.mol
Determination of sublimation enthalpies of substituted benzophenones, fluorenes and diphenyl ethers by solution calorimetry approach:	https://www.doi.org/10.1016/j.tca.2017.08.003
ChemEo Relay (1.0):	
ChemEo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids:	https://www.doi.org/10.1016/j.jct.2012.02.001
Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures:	https://www.doi.org/10.1016/j.jct.2015.09.028
Standard enthalpy of formation of diphenyl oxide:	https://www.doi.org/10.1016/j.jct.2018.04.009
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Benchmark properties of diphenyl oxide as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2018.05.021
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity

dm:	Dipole Moment
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume