

# Diphenyl ether

**Other names:** 1,1'-OXYBIS-BENZENE  
1,1'-Oxybisbenzene  
BIPHENYL OXIDE  
Benzene, 1,1'-oxybis-  
Benzene, phenoxy-  
Chemcrys JK-EB  
Diphenyl oxide  
Ether, diphenyl-  
Geranium crystals  
NSC 19311  
Oxybisbenzene  
Oxydiphenyl  
PHENOXY BENZENE  
Phenoxybenzene  
Phenyl ether  
Phenyl oxide

**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	65.00	kJ/mol	NIST Webbook
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	67.10	kJ/mol	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.09 ± 0.03	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
ie	8.00	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	1381.70		NIST Webbook
rinpol	241.16		NIST Webbook
rinpol	241.70		NIST Webbook
rinpol	241.70		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1366.40		NIST Webbook
rinpol	1389.90		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1376.30		NIST Webbook
rinpol	1366.80		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.90		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1376.20		NIST Webbook
rinpol	1371.80		NIST Webbook
rinpol	1384.60		NIST Webbook
rinpol	1372.60		NIST Webbook
rinpol	1356.90		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1396.00		NIST Webbook

rinpol	1372.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1380.10		NIST Webbook
rinpol	1393.70		NIST Webbook
rinpol	1366.40		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2026.00		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	788.15 ± 2.00	K	NIST Webbook
tc	767.20 ± 1.00	K	NIST Webbook
tc	766.80 ± 1.00	K	NIST Webbook
tf	300.00 ± 0.02	K	NIST Webbook
tf	299.90 ± 0.02	K	NIST Webbook
tf	300.15 ± 1.00	K	NIST Webbook
tf	300.05 ± 0.05	K	NIST Webbook
tf	299.90 ± 0.40	K	NIST Webbook
tf	299.90 ± 0.30	K	NIST Webbook
tf	300.02	K	KDB
tf	300.60	K	Aqueous Solubility Prediction Method
tf	300.58 ± 0.20	K	NIST Webbook
tf	300.04 ± 0.01	K	NIST Webbook
tf	300.20 ± 0.20	K	NIST Webbook
tt	300.01 ± 0.00	K	NIST Webbook
tt	300.03 ± 0.01	K	NIST Webbook
vc	0.509	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.51	J/mol×K	754.88	Joback Method
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	380.90	J/mol×K	795.91	Joback Method
cps	216.56	J/mol×K	298.15	NIST Webbook
cps	216.56	J/mol×K	298.15	NIST Webbook
cps	215.90	J/mol×K	298.50	NIST Webbook
dvisc	0.0001694	Paxs	549.74	Joback Method
dvisc	0.0002159	Paxs	508.13	Joback Method
dvisc	0.0004047	Paxs	424.91	Joback Method
dvisc	0.0019947	Paxs	300.07	Joback Method
dvisc	0.0006136	Paxs	383.29	Joback Method
dvisc	0.0010297	Paxs	341.68	Joback Method
dvisc	0.0002874	Paxs	466.52	Joback Method
hfust	17.21	kJ/mol	300.03	NIST Webbook
hfust	17.22	kJ/mol	300.02	NIST Webbook
hfust	16.51	kJ/mol	300.40	NIST Webbook
hfust	17.21	kJ/mol	300.00	NIST Webbook
hfust	17.21	kJ/mol	300.00	NIST Webbook
hvapt	64.20	kJ/mol	323.00	NIST Webbook
hvapt	53.00	kJ/mol	510.50	NIST Webbook
hvapt	48.20	kJ/mol	510.50	NIST Webbook
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	0.04	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	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	0.03	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	0.09	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
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	0.02	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	0.01	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	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	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	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	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	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	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	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

rhol	1066.00	kg/m3	303.00	KDB
rhol	1061.20	kg/m3	308.15	Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures
rhol	1039.60	kg/m3	333.15	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	1022.30	kg/m3	353.15	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	1005.20	kg/m3	373.15	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	1056.90	kg/m3	313.15	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
sfust	57.38	J/mol×K	300.02	NIST Webbook
sfust	57.38	J/mol×K	300.03	NIST Webbook
tcondl	0.13	W/m×K	303.15	Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids
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

## Correlations

Information	Value
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Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/(T + C)$
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

**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>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as azeotropic solvents:** <https://www.doi.org/10.1016/j.jct.2012.02.001>  
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C101848&Units=SI>

**Standard enthalpy of formation of diphenyl oxide:** <https://www.doi.org/10.1016/j.jct.2018.04.009>  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

**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 KDP carrier: Evaluation of thermochemical data with complementary experimental and computational methods:** <https://www.doi.org/10.1016/j.jct.2018.05.021>

<https://www.cheric.org/files/research/kdb/mol/mol1031.mol>

## Legend

<b>af:</b>	Acentric Factor
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>nfpaf:</b>	NFPA Fire Rating
<b>nfpah:</b>	NFPA Health Rating
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhol:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tcondl:</b>	Liquid thermal conductivity
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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