o-Terphenyl

Other names:	1,1'-Biphenyl, 2-phenyl-
	1,1':2',1''-Terphenyl
	1,2-DIPHENYLBENZENE
	1,2-terphenyl
	2-PHENYL-1,1'-BIPHENYL
	2-Phenylbiphenyl
	benzene, 1,2-diphenyl-
Inchi:	InChI=1S/C18H14/c1-3-9-15(10-4-1)17-13-7-8-14-18(17)16-11-5-2-6-12-16/h1-14H
InchiKey:	OIAQMFOKAXHPNH-UHFFFAOYSA-N
Formula:	C18H14
SMILES:	c1ccc(-c2ccccc2-c2ccccc2)cc1
Mol. weight [g/mol]:	230.30
CAS:	84-15-1

Physical Properties

Property code	Value	Unit	Source
af	0.4310		KDB
gf	428.28	kJ/mol	Joback Method
hf	282.80 ± 3.20	kJ/mol	NIST Webbook
hfs	179.80 ± 3.10	kJ/mol	NIST Webbook
hfus	24.11	kJ/mol	Joback Method
hsub	97.00 ± 1.00	kJ/mol	NIST Webbook
hsub	103.00 ± 0.40	kJ/mol	NIST Webbook
hsub	103.00 ± 0.80	kJ/mol	NIST Webbook
hvap	84.20 ± 0.40	kJ/mol	NIST Webbook
ie	8.43	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.64 ± 0.05	eV	NIST Webbook
ie	7.99 ± 0.01	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	7.99 ± 0.01	eV	NIST Webbook
log10ws	-6.68		Crippen Method
logp	5.021		Crippen Method
mcvol	193.200	ml/mol	McGowan Method
pc	2990.00	kPa	KDB
pc	3000.00 ± 600.00	kPa	NIST Webbook
pc	2990.00 ± 607.95	kPa	NIST Webbook

pc	3500.00 ± 689.50	kPa	NIST Webbook
rhoc	315.52 ± 20.04	kg/m3	NIST Webbook
rhoc	322.43 ± 138.18	kg/m3	NIST Webbook
rhoc	306.30 ± 29.94	kg/m3	NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	317.43		NIST Webbook
rinpol	316.63		NIST Webbook
rinpol	321.99		NIST Webbook
rinpol	317.43		NIST Webbook
rinpol	321.70		NIST Webbook
rinpol	317.42		NIST Webbook
rinpol	1886.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1910.10		NIST Webbook
rinpol	316.63		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	321.99		NIST Webbook
ripol	2649.00		NIST Webbook
ripol	2649.00		NIST Webbook
sl	337.11	J/mol×K	NIST Webbook
ss	298.81	J/mol×K	NIST Webbook
tb	610.20	K	NIST Webbook
tb	605.20	K	NIST Webbook
tb	455.00 ± 25.00	K	NIST Webbook
tb	605.00	K	KDB
tc	857.00 ± 5.00	K	NIST Webbook
tc	890.90 ± 16.70	K	NIST Webbook
tc	857.00	K	KDB
tc	857.00 ± 6.00	K	NIST Webbook
tf	332.00 ± 3.00	K	NIST Webbook
tf	329.90 ± 2.00	K	NIST Webbook
tf	329.60 ± 4.00	K	NIST Webbook
tf	331.00 ± 3.00	K	NIST Webbook
tf	330.00 ± 3.00	K	NIST Webbook
tf	329.30	K	KDB
tf	331.15 ± 1.00	K	NIST Webbook
tt	329.35 ± 0.01	K	NIST Webbook

tt	270.00	K	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
tt	329.40	K	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
vc	0.731	m3/kmol	NIST Webbook
vc	0.731	m3/kmol	KDB
zc	0.3067400		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.66	J/mol×K	876.42	Joback Method
cpg	570.80	J/mol×K	921.46	Joback Method
cpg	496.03	J/mol×K	696.26	Joback Method
cpg	514.08	J/mol×K	741.30	Joback Method
cpg	530.44	J/mol×K	786.34	Joback Method
cpg	545.25	J/mol×K	831.38	Joback Method
cpg	581.81	J/mol×K	966.50	Joback Method
cpl	369.05	J/mol×K	298.15	NIST Webbook
cps	274.73	J/mol×K	298.15	Reassembling and testing of a high-precision heat capacity drop calorimeter. Heat capacity of some polyphenyls at T = 298.15 K
cps	274.75	J/mol×K	298.15	NIST Webbook
dvisc	0.0001578	Pa×s	644.28	Joback Method
dvisc	0.0001244	Pa×s	696.26	Joback Method
dvisc	0.0013626	Pa×s	384.40	Joback Method
dvisc	0.0007210	Pa×s	436.38	Joback Method
dvisc	0.0004368	Pa×s	488.35	Joback Method
dvisc	0.0002915	Pa×s	540.33	Joback Method
dvisc	0.0002088	Pa×s	592.31	Joback Method
hfust	17.20	kJ/mol	329.40	NIST Webbook
hfust	17.20	kJ/mol	329.40	NIST Webbook
hfust	17.19	kJ/mol	329.35	NIST Webbook

hfust	16.90	kJ/mol	327.80	NIST Webbook
hfust	17.20	kJ/mol	328.40	NIST Webbook
hvapt	77.60	kJ/mol	402.50	NIST Webbook
hvapt	68.50	kJ/mol	556.00	NIST Webbook
hvapt	81.00 ± 0.40	kJ/mol	351.50	NIST Webbook
hvapt	60.50	kJ/mol	681.00	NIST Webbook
rhos	1120.00	kg/m3	298.15	Standard molar enthalpies of formation and of sublimation of the terphenyl isomers
sfust	52.30	J/mol×K	329.40	NIST Webbook
sfust	52.20	J/mol×K	329.35	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74653e+01
Coeff. B	-6.38564e+03
Coeff. C	-8.33970e+01
Temperature range (K), min.	455.15
Temperature range (K), max.	609.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02099e+02
Coeff. B	-1.32293e+04
Coeff. C	-1.20005e+01
Coeff. D	3.15381e-06
Temperature range (K), min.	329.35
Temperature range (K), max.	890.95

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol808.mol

Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series:	https://www.doi.org/10.1016/j.jct.2013.03.026
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds. Fast-crystallizing m-terphenyl:	https://www.doi.org/10.1016/j.tca.2018.08.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Heat capacities in a deeply supercooled liquid state:	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=808
Reassembling and testing of a high-precision heat capacity drop calorimeter:	https://www.doi.org/10.1016/j.jct.2011.06.010
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Heat capacity of some polyphenyls at T = 298.15 K:	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84151&Units=SI
Standard molar enthalpies of formation and of sublimation of the terphenyl isomers:	https://www.doi.org/10.1016/j.jct.2007.08.008

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
rhoc:	Critical density
rhos:	Solid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
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
vc:	Critical Volume
zc:	Critical Compressibility