m-Terphenyl

Other names:	1,1'-Biphenyl, 3-phenyl- 1,1':3',1''-Terphenyl 1,3-DIPHENYLBENZENE 1,3-Terphenyl 3-Phenyl-1,1'-biphenyl 3-Phenylbiphenyl Benzene, m-diphenyl- ISODIPHENYLBENZENE NSC 6808 SANTOWAX M benzene, 1,3-diphenyl- m-Diphenylbenzene m-Triphenyl
Inchi:	InChI=1S/C18H14/c1-3-8-15(9-4-1)17-12-7-13-18(14-17)16-10-5-2-6-11-16/h1-14H
InchiKey:	YJTKZCDBKVTVBY-UHFFFAOYSA-N
Formula:	C18H14
SMILES:	c1ccc(-c2cccc(-c3ccccc3)c2)cc1
Mol. weight [g/mol]:	230.30
CAS:	92-06-8

Physical Properties

Property code	Value	Unit	Source
af	0.4490		KDB
gf	428.28	kJ/mol	Joback Method
hf	280.00 ± 3.90	kJ/mol	NIST Webbook
hfs	161.60 ± 3.10	kJ/mol	NIST Webbook
hfus	24.11	kJ/mol	Joback Method
hsub	118.40 ± 2.40	kJ/mol	NIST Webbook
hsub	118.10 ± 1.60	kJ/mol	NIST Webbook
hsub	120.00 ± 1.00	kJ/mol	NIST Webbook
hsub	118.60 ± 0.70	kJ/mol	NIST Webbook
hvap	97.20 ± 0.30	kJ/mol	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	8.80 ± 0.05	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.02 ± 0.10	eV	NIST Webbook
ie	8.01 ± 0.01	eV	NIST Webbook

log10ws	-6.68		Crippen Method
logp	5.021		Crippen Method
mcvol	193.200	ml/mol	McGowan Method
pc	2480.00 ± 506.62	kPa	NIST Webbook
pc	2500.00 ± 500.00	kPa	NIST Webbook
pc	2480.00	kPa	KDB
pc	3500.00 ± 689.50	kPa	NIST Webbook
rhoc	317.82 ± 20.04	kg/m3	NIST Webbook
rhoc	322.43 ± 115.15	kg/m3	NIST Webbook
rhoc	299.39 ± 29.94	kg/m3	NIST Webbook
rinpol	360.73		NIST Webbook
rinpol	360.73		NIST Webbook
rinpol	351.70		NIST Webbook
rinpol	2164.00		NIST Webbook
rinpol	358.30		NIST Webbook
rinpol	356.74		NIST Webbook
rinpol	2142.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	356.12		NIST Webbook
rinpol	352.60		NIST Webbook
tb	652.20	K	NIST Webbook
tb	636.00	K	KDB
tc	883.00 ± 10.00	K	NIST Webbook
tc	924.80 ± 16.70	K	NIST Webbook
tc	883.00	K	KDB
tc	883.00 ± 10.00	K	NIST Webbook
tf	361.00	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
tf	360.00	K	KDB
tt	361.80	K	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
vc	0.724	m3/kmol	NIST Webbook
vc	0.724	m3/kmol	KDB
zc	0.2445640		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	558.66	J/mol×K	876.42	Joback Method
cpg	581.81	J/mol×K	966.50	Joback Method
cpl	417.10	J/mol×K	370.00	NIST Webbook
cps	277.42	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
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
dvisc	0.0001578	Pa×s	644.28	Joback Method
hfust	22.59	kJ/mol	360.00	NIST Webbook
hfust	31.00	kJ/mol	361.20	NIST Webbook
hsubt	119.00	kJ/mol	338.00	NIST Webbook
hsubt	115.50 ± 1.60	kJ/mol	341.00	NIST Webbook
hvapt	76.10	kJ/mol	576.50	NIST Webbook
rhos	1140.00	kg/m3	298.15	Standard molar enthalpies of formation and of sublimation of the terphenyl isomers

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.33779e+01
Coeff. B	-9.23410e+03
Coeff. C	-8.82170e+01
Temperature range (K), min.	488.15
Temperature range (K), max.	599.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.22524e+02
Coeff. B	-1.54842e+04
Coeff. C	-1.47697e+01
Coeff. D	3.78520e-06
Temperature range (K), min.	360.00
Temperature range (K), max.	924.85

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol809.mol
Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds. Fast-crystallizing supercooled liquid state:	https://www.doi.org/10.1016/j.tca.2018.08.015
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=809
Standard molar enthalpies of formation and of sublimation of the terphenyl isomers at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2007.08.008
Liquid phase heat capacities in a deeply supercooled liquid state:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92068&Units=SI
NIST Webbook	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Reassembling and testing of a high-precision heat capacity drop calorimeter. Heat capacity of some oligophenyls at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.06.010
Isomerization effect on the heat capacities and phase behavior of oligophenyls. Isomers series:	https://www.doi.org/10.1016/j.jct.2013.03.026
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

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
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
rhoc:	Critical density
rhos:	Solid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility