1,1':4',1'':4'',1'''-Quaterphenyl

Other names:	1,1'-biphenyl, 4,4'-diphenyl-
	4,4'-diphenylbiphenyl
	Quadriphenyl
	benzerythrene
	p,p'-Quaterphenyl
	p-quaterphenyl
	p-tetraphenyl
Inchi:	InChI=1S/C24H18/c1-3-7-19(8-4-1)21-11-15-23(16-12-21)24-17-13-22(14-18-24)20-9-5-2
InchiKey:	GPRIERYVMZVKTC-UHFFFAOYSA-N
Formula:	C24H18
SMILES:	c1ccc(-c2ccc(-c3ccc(-c4ccccc4)cc3)cc2)cc1
Mol. weight [g/mol]:	306.40
CAS:	135-70-6

Physical Properties

Property code	Value	Unit	Source
chs	-12244.00 ± 6.30	kJ/mol	NIST Webbook
ea	0.66 ± 0.02	eV	NIST Webbook
gf	581.58	kJ/mol	Joback Method
hf	400.00 ± 11.00	kJ/mol	NIST Webbook
hf	382.00 ± 7.50	kJ/mol	NIST Webbook
hfs	227.00 ± 6.30	kJ/mol	NIST Webbook
hfs	227.00 ± 7.00	kJ/mol	NIST Webbook
hfus	33.30	kJ/mol	Joback Method
hsub	155.00	kJ/mol	NIST Webbook
hsub	172.50 ± 8.40	kJ/mol	NIST Webbook
hsub	156.00 ± 1.00	kJ/mol	NIST Webbook
hvap	136.10 ± 1.60	kJ/mol	NIST Webbook
ie	8.08 ± 0.05	eV	NIST Webbook
log10ws	-9.28		Crippen Method
logp	6.688		Crippen Method
mcvol	253.980	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	472.80		NIST Webbook
rinpol	472.81		NIST Webbook
rinpol	488.18		NIST Webbook
rinpol	488.18		NIST Webbook

ss	363.64	J/mol×K	NIST Webbook
tb	865.20	K	Joback Method
tc	1146.33	K	Joback Method
tf	586.70 ± 0.50	K	NIST Webbook
tf	581.60 ± 4.00	K	NIST Webbook
tf	587.20 ± 0.50	K	NIST Webbook
tf	591.00 ± 4.00	K	NIST Webbook
tf	576.00 ± 2.00	K	NIST Webbook
tt	594.40	K	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.64	J/mol×K	1146.33	Joback Method
cpg	791.51	J/mol×K	1052.62	Joback Method
cpg	749.87	J/mol×K	912.06	Joback Method
cpg	732.93	J/mol×K	865.20	Joback Method
cpg	765.15	J/mol×K	958.91	Joback Method
cpg	778.96	J/mol×K	1005.77	Joback Method
cpg	803.00	J/mol×K	1099.48	Joback Method
cps	340.00	J/mol×K	300.00	NIST Webbook
cps	362.52	J/mol×K	298.15	NIST Webbook
cps	363.45	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	0.0001500	Pa×s	678.08	Joback Method
dvisc	0.0000654	Pa×s	865.20	Joback Method
dvisc	0.0000827	Pa×s	802.83	Joback Method
dvisc	0.0006475	Pa×s	490.96	Joback Method
dvisc	0.0003563	Pa×s	553.33	Joback Method
dvisc	0.0002213	Pa×s	615.71	Joback Method
dvisc	0.0001086	Pa×s	740.45	Joback Method
hfust	37.80	kJ/mol	587.20	NIST Webbook
hfust	37.80	kJ/mol	587.20	NIST Webbook
hfust	57.60	kJ/mol	586.70	NIST Webbook

pvap	8.99e-03	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.87e-03	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.54e-03	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.12	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.27e-03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.07e-04	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.76e-04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.19e-04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.81e-05	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.83e-05	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	6.49e-06	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.13e-06	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.44e-07	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.77e-07	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.41e-08	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.84e-09	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.94e-09	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	3.35e-10	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.38e-10	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
sfust	98.20	J/mol×K	586.70	NIST Webbook
sfust	64.40	J/mol×K	587.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	701.20	K	2.40	NIST Webbook

Sources

Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series:	https://www.doi.org/10.1016/j.jct.2013.03.026
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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 polyphenyls at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.06.010

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume