

1,1':4',1'':4'',1''':4'''-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	156.00 ± 1.00	kJ/mol	NIST Webbook
hsub	172.50 ± 8.40	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
mvol	253.980	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	472.80		NIST Webbook
rinpol	488.18		NIST Webbook
rinpol	472.81		NIST Webbook
rinpol	488.18		NIST Webbook

ss	363.64	J/molxK	NIST Webbook
tb	865.20	K	Joback Method
tc	1146.33	K	Joback Method
tf	587.20 ± 0.50	K	NIST Webbook
tf	586.70 ± 0.50	K	NIST Webbook
tf	591.00 ± 4.00	K	NIST Webbook
tf	581.60 ± 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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.87	J/molxK	912.06	Joback Method
cpg	765.15	J/molxK	958.91	Joback Method
cpg	778.96	J/molxK	1005.77	Joback Method
cpg	791.51	J/molxK	1052.62	Joback Method
cpg	803.00	J/molxK	1099.48	Joback Method
cpg	813.64	J/molxK	1146.33	Joback Method
cpg	732.93	J/molxK	865.20	Joback Method
cps	363.45	J/molxK	298.15	Reassembling and testing of a high-precision heat capacity drop calorimeter. Heat capacity of some polyphenyls at T = 298.15 K
cps	340.00	J/molxK	300.00	NIST Webbook
cps	362.52	J/molxK	298.15	NIST Webbook
dvisc	0.0000654	Paxs	865.20	Joback Method
dvisc	0.0000827	Paxs	802.83	Joback Method
dvisc	0.0001086	Paxs	740.45	Joback Method
dvisc	0.0001500	Paxs	678.08	Joback Method
dvisc	0.0002213	Paxs	615.71	Joback Method
dvisc	0.0003563	Paxs	553.33	Joback Method
dvisc	0.0006475	Paxs	490.96	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	2.13e-06	kPa	360.00	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	6.44e-07	kPa	350.00	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	1.27e-03	kPa	430.00	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	4.87e-03	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	8.99e-03	kPa	460.00	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	0.03	kPa	480.00	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	0.07	kPa	500.00	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	1.77e-07	kPa	340.00	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	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
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	2.76e-04	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
sfust	98.20	J/molxK	586.70	NIST Webbook
sfust	64.40	J/molxK	587.20	NIST Webbook

Pressure Dependent Properties

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

Sources

Reassembling and testing of a high-precision heat capacity drop calorimeter. Effect on the heat capacities and phase behavior of hydrocarbons. Isomer-specific Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons: McGowan Method:

<https://www.doi.org/10.1016/j.jct.2011.06.010>

<https://www.doi.org/10.1016/j.jct.2013.03.026>

<https://www.doi.org/10.1021/je800300x>

https://en.wikipedia.org/wiki/Joback_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/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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

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