

# 1,1':4',1":4",1''':4''',1''''-Quinquephenyl

Other names:

p-Pentaphenyl  
p-Quinquiphenyl  
p-quinquephenyl

Inchi:

InChI=1S/C30H22/c1-3-7-23(8-4-1)25-11-15-27(16-12-25)29-19-21-30(22-20-29)28-17-1

InchiKey:

OMCUOJTVNIHQTI-UHFFFAOYSA-N

Formula:

C30H22

SMILES:

c1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccccc5)cc4)cc3)cc2)cc1

Mol. weight [g/mol]:

382.50

CAS:

3073-05-0

## Physical Properties

Property code	Value	Unit	Source
gf	734.88	kJ/mol	Joback Method
hf	485.71	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	95.74	kJ/mol	Joback Method
ie	8.18 ± 0.05	eV	NIST Webbook
log10ws	-11.88		Crippen Method
logp	8.355		Crippen Method
mcvol	314.760	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	1034.14	K	Joback Method
tc	1323.15	K	Joback Method
tf	645.00 ± 6.00	K	NIST Webbook
vc	1.175	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.19	J/molxK	1274.98	Joback Method
cpg	976.86	J/molxK	1034.14	Joback Method
cpg	991.89	J/molxK	1082.31	Joback Method
cpg	1005.67	J/molxK	1130.48	Joback Method
cpg	1018.47	J/molxK	1178.64	Joback Method

cpg	1030.55	J/molxK	1226.81	Joback Method
cpg	1053.65	J/molxK	1323.15	Joback Method
cps	455.50	J/molxK	298.15	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
dvisc	0.0000317	Paxs	1034.14	Joback Method
dvisc	0.0002934	Paxs	597.52	Joback Method
dvisc	0.0001656	Paxs	670.29	Joback Method
dvisc	0.0001045	Paxs	743.06	Joback Method
dvisc	0.0000716	Paxs	815.83	Joback Method
dvisc	0.0000522	Paxs	888.60	Joback Method
dvisc	0.0000399	Paxs	961.37	Joback Method
hfust	42.30	kJ/mol	659.60	NIST Webbook
sfust	64.10	J/molxK	659.60	NIST Webbook

## Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series:**

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

[https://en.wikipedia.org/wiki/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=C3073050&Units=SI>

**Crippen Method:**

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

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	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>hvac:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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