

1,1':2',1":2",1""-Quaterphenyl

Other names:	1,1'-Biphenyl, 2,2'-diphenyl- 2,2'-diphenyl-1,1'-biphenyl 2,2'-diphenylbiphenyl O,O-Quaterphenyl o,o'-quaterphenyl o-quaterphenyl ortho-Quaterphenyl
Inchi:	InChI=1S/C24H18/c1-3-11-19(12-4-1)21-15-7-9-17-23(21)24-18-10-8-16-22(24)20-13-5-
InchiKey:	YAVCXSHORWKJQQ-UHFFFAOYSA-N
Formula:	C24H18
SMILES:	<chem>c1ccc(-c2ccccc2-c2ccccc2-c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	306.40
CAS:	641-96-3

Physical Properties

Property code	Value	Unit	Source
gf	581.58	kJ/mol	Joback Method
hf	384.49	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
ie	8.52 ± 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	423.63		NIST Webbook
rinpol	423.63		NIST Webbook
rinpol	423.63		NIST Webbook
rinpol	423.63		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	394.68		NIST Webbook
tb	693.20	K	NIST Webbook
tc	1146.33	K	Joback Method
tf	490.96	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.64	J/molxK	1146.33	Joback Method
cpg	803.00	J/molxK	1099.48	Joback Method
cpg	791.51	J/molxK	1052.62	Joback Method
cpg	778.96	J/molxK	1005.77	Joback Method
cpg	765.15	J/molxK	958.91	Joback Method
cpg	749.87	J/molxK	912.06	Joback Method
cpg	732.93	J/molxK	865.20	Joback Method
cps	359.10	J/molxK	298.15	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
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
dvisc	0.0000654	Paxs	865.20	Joback Method

Sources

Crippen Method:

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

Crippen Method:

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>

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=C641963&Units=SI>

Legend

cpg: Ideal gas heat capacity

cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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