

1,1':4',1":4",1"":4"",1""":4""",1""":4"""-Sexiphenyl

Other names:	p-Quaterphenyl, 4,4""-diphenyl- p-Sexiphenyl 1,1':4',1":4",1""-Quaterphenyl, 4,4""-diphenyl- p-Hexaphenyl p-Sexiphenylene
Inchi:	InChI=1S/C36H26/c1-3-7-27(8-4-1)29-11-15-31(16-12-29)33-19-23-35(24-20-33)36-25-2
InchiKey:	ZEMDSNVUUOCIED-UHFFFAOYSA-N
Formula:	C36H26
SMILES:	c1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(-c6ccccc6)cc5)cc4)cc3)cc2)cc1
Mol. weight [g/mol]:	458.59
CAS:	4499-83-6

Physical Properties

Property code	Value	Unit	Source
gf	888.18	kJ/mol	Joback Method
hf	586.93	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	112.03	kJ/mol	Joback Method
ie	7.67 ± 0.05	eV	NIST Webbook
log10ws	-14.49		Crippen Method
logp	10.022		Crippen Method
mcvol	375.540	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
tb	1203.08	K	Joback Method
tc	1502.25	K	Joback Method
tf	704.08	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.68	J/molxK	1203.08	Joback Method
cpg	1238.09	J/molxK	1252.94	Joback Method
cpg	1252.09	J/molxK	1302.80	Joback Method

cpg	1266.01	J/molxK	1352.66	Joback Method
cpg	1280.21	J/molxK	1402.52	Joback Method
cpg	1295.04	J/molxK	1452.38	Joback Method
cpg	1310.85	J/molxK	1502.25	Joback Method
dvisc	0.0001288	Paxs	704.08	Joback Method
dvisc	0.0000740	Paxs	787.25	Joback Method
dvisc	0.0000473	Paxs	870.41	Joback Method
dvisc	0.0000326	Paxs	953.58	Joback Method
dvisc	0.0000239	Paxs	1036.75	Joback Method
dvisc	0.0000184	Paxs	1119.91	Joback Method
dvisc	0.0000146	Paxs	1203.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4499836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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