Hexaphenylbenzene

Other names:	Benzene, hexaphenyl- 1,1':2',1''-Terphenyl, 3',4',5',6'-tetraphenyl- m-Terphenyl, 2',4',5',6'-tetraphenyl- 3',4',5',6'-tetraphenyl-o-terphenyl
Inchi:	InChI=1S/C42H30/c1-7-19-31(20-8-1)37-38(32-21-9-2-10-22-32)40(34-25-13-4-14-26-34
InchiKey:	QBHWPVJPWQGYDS-UHFFFAOYSA-N
Formula:	C42H30
SMILES:	c1ccc(-c2c(-c3ccccc3)c(-c3ccccc3)c(-c3ccccc3)c(-c3ccccc3)c2-c2ccccc2)cc1
Mol. weight [g/mol]:	534.69
CAS:	992-04-1

Physical Properties

Property code	Value	Unit	Source
gf	1041.48	kJ/mol	Joback Method
hf	688.15	kJ/mol	Joback Method
hfus	60.88	kJ/mol	Joback Method
hvap	128.33	kJ/mol	Joback Method
ie	8.47 ± 0.05	eV	NIST Webbook
log10ws	-17.09		Crippen Method
logp	11.689		Crippen Method
mcvol	436.320	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
tb	1372.02	K	Joback Method
tc	1688.44	K	Joback Method
tf	810.64	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.57	J/mol×K	1372.02	Joback Method
cpg	1579.28	J/mol×K	1635.71	Joback Method
cpg	1555.08	J/mol×K	1582.97	Joback Method
cpg	1533.29	J/mol×K	1530.23	Joback Method

cpg	1513.42	J/mol×K	1477.49	Joback Method
cpg	1495.01	J/mol×K	1424.76	Joback Method
cpg	1606.36	J/mol×K	1688.44	Joback Method
dvisc	0.0000065	Pa×s	1372.02	Joback Method
dvisc	0.0000081	Pa×s	1278.46	Joback Method
dvisc	0.0000106	Pa×s	1184.89	Joback Method
dvisc	0.0000144	Pa×s	1091.33	Joback Method
dvisc	0.0000207	Pa×s	997.77	Joback Method
dvisc	0.0000322	Pa×s	904.20	Joback Method
dvisc	0.0000553	Pa×s	810.64	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C992041&Units=SI

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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