1,1'-Biphenyl, 4-(4-pentylcyclohexyl)-4'-(4-propylcyclohexyl)-

Other names: 1,1'-Biphenyl, 4-(4-pentylcyclohexyl)-4'-(4-propylcyclohexyl)-
[trans(trans)]-4-(4-pentylcyclohexyl)-4'-(4-propylcyclohexyl)biphenyl
[trans(trans)]-4-(4-pentylcyclohexyl)-4'-(4-propylcyclohexyl)-1,1'-biphenyl

Inchi: InChI=1S/C32H46/c1-3-5-6-8-26-11-15-28(16-12-26)30-19-23-32(24-20-30)31-21-17-29(

InchiKey: PJBOOKMLDPERRS-UHFFFAOYSA-N

Formula: C32H46

SMILES: CCCCCC1CCC(c2ccc(-c3ccc(C4CCC(CCC)CC4)cc3)cc2)CC1

Mol. weight [g/mol]: 430.72

Physical Properties

Property code	Value	Unit	Source
af	0.8169		Cheméo Relay (1.0)
gf	457.60	kJ/mol	Joback Method
hf	-183.64	kJ/mol	Cheméo Relay (1.0)
hfus	51.75	kJ/mol	Joback Method
hvap	144.33	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-10.19		Cheméo Relay (1.0)
logp	10.282		Crippen Method
mcvol	392.500	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
tb	785.63	K	Cheméo Relay (1.0)
tc	997.15	K	Cheméo Relay (1.0)
tf	401.20	K	Cheméo Relay (1.0)
vc	1.438	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.10	J/mol×K	1024.64	Joback Method
cpg	1444.52	J/mol×K	1065.00	Joback Method
cpg	1462.88	J/mol×K	1105.36	Joback Method
cpg	1479.32	J/mol×K	1145.73	Joback Method
cpg	1493.96	J/mol×K	1186.09	Joback Method

cpg	1506.94	J/mol×K	1226.45	Joback Method
cpg	1518.40	J/mol×K	1266.81	Joback Method
dvisc	0.0005946	Pa×s	534.56	Joback Method
dvisc	0.0002797	Pa×s	616.24	Joback Method
dvisc	0.0001570	Pa×s	697.92	Joback Method
dvisc	0.0000995	Pa×s	779.60	Joback Method
dvisc	0.0000687	Pa×s	861.28	Joback Method
dvisc	0.0000506	Pa×s	942.96	Joback Method
dvisc	0.0000391	Pa×s	1024.64	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80955711&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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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