1,1'-Biphenyl, 2,2',4,4',5,5'-hexabromo-

Other names:	2,2',4,4',5,5'-Hexabromo-1,1'-biphenyl
	2,2',4,4',5,5'-Hexabromobiphenyl
	2,4,5,2',4',5'-Hexabromobiphenyl
Inchi:	InChI=1S/C12H4Br6/c13-7-3-11(17)9(15)1-5(7)6-2-10(16)12(18)4-8(6)14/h1-4H
InchiKey:	HMBBJSKXDBUNNT-UHFFFAOYSA-N
Formula:	C12H4Br6
SMILES:	Brc1cc(Br)c(-c2cc(Br)c(Br)cc2Br)cc1Br
Mol. weight [g/mol]:	627.58
CAS:	59080-40-9

Physical Properties

Property code	Value	Unit	Source
gf	303.12	kJ/mol	Joback Method
hf	271.21	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	89.44	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	7.929		Crippen Method
mcvol	237.420	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
tb	954.16	K	Joback Method
tc	1269.63	K	Joback Method
tf	711.76	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.26	J/mol×K	954.16	Joback Method
cpg	438.47	J/mol×K	1006.74	Joback Method
cpg	445.68	J/mol×K	1059.32	Joback Method
cpg	453.10	J/mol×K	1111.90	Joback Method
cpg	460.94	J/mol×K	1164.47	Joback Method
cpg	469.41	J/mol×K	1217.05	Joback Method

cpg	478.71	J/mol×K	1269.63	Joback Method
dvisc	0.0002217	Pa×s	711.76	Joback Method
dvisc	0.0001780	Pa×s	752.16	Joback Method
dvisc	0.0001462	Pa×s	792.56	Joback Method
dvisc	0.0001224	Pa×s	832.96	Joback Method
dvisc	0.0001041	Pa×s	873.36	Joback Method
dvisc	0.0000899	Pa×s	913.76	Joback Method
dvisc	0.0000785	Pa×s	954.16	Joback Method

Sources

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=C59080409&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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