2,2',4,4',6,6'-Hexabromobiphenyl

Other names: 2,2',4,4',6,6'-Hexabromo-1,1'-biphenyl
Inchi: InChI=1S/C12H4Br6/c13-5-1-7(15)11(8(16)2-5)12-9(17)3-6(14)4-10(12)18/h1-4H
InchiKey: LNFYSRMCCKKDEH-UHFFFAOYSA-N
Formula: C12H4Br6
SMILES: Brc1cc(Br)c(-c2c(Br)cc(Br)cc2Br)c(Br)c1
Mol. weight [g/mol]: 627.58
CAS: 59261-08-4

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	469.41	J/mol×K	1217.05	Joback Method
cpg	460.94	J/mol×K	1164.47	Joback Method
cpg	453.10	J/mol×K	1111.90	Joback Method
cpg	445.68	J/mol×K	1059.32	Joback Method
cpg	438.47	J/mol×K	1006.74	Joback Method
cpg	478.71	J/mol×K	1269.63	Joback Method
dvisc	0.0000785	Pa×s	954.16	Joback Method

dvisc	0.0000899	Pa×s	913.76	Joback Method
dvisc	0.0001041	Pa×s	873.36	Joback Method
dvisc	0.0001224	Pa×s	832.96	Joback Method
dvisc	0.0001462	Pa×s	792.56	Joback Method
dvisc	0.0001780	Pa×s	752.16	Joback Method
dvisc	0.0002217	Pa×s	711.76	Joback Method

Sources

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=C59261084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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