2,2',4,4',5,5'-Hexabromodiphenyl ether

Other names: BDE-153
Inchi: InChI=1S/C12H4Br6O/c13-5-1-9(17)11(3-7(5)15)19-12-4-8(16)6(14)2-10(12)18/h1-4H
InchiKey: RZXIRSKYBISPGF-UHFFFAOYSA-N
Formula: C12H4Br6O
SMILES: Brc1cc(Br)c(Oc2cc(Br)c(Br)cc2Br)cc1Br
Mol. weight [g/mol]: 643.58
CAS: 68631-49-2

Physical Properties

Property code	Value	Unit	Source
gf	198.12	kJ/mol	Joback Method
hf	138.99	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	91.85	kJ/mol	Joback Method
log10ws	-10.08		Crippen Method
logp	8.054		Crippen Method
mcvol	243.290	ml/mol	McGowan Method
pc	5094.76	kPa	Joback Method
tb	976.58	K	Joback Method
tc	1285.26	K	Joback Method
tf	733.99	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.95	J/mol×K	976.58	Joback Method
cpg	466.18	J/mol×K	1079.47	Joback Method
cpg	492.95	J/mol×K	1285.26	Joback Method
cpg	472.61	J/mol×K	1130.92	Joback Method
cpg	479.11	J/mol×K	1182.37	Joback Method
cpg	485.84	J/mol×K	1233.82	Joback Method
cpg	459.68	J/mol×K	1028.03	Joback Method
dvisc	0.0000661	Pa×s	936.15	Joback Method

dvisc	0.0000765	Pa×s	895.72	Joback Method
dvisc	0.0000898	Pa×s	855.29	Joback Method
dvisc	0.0001071	Pa×s	814.85	Joback Method
dvisc	0.0001300	Pa×s	774.42	Joback Method
dvisc	0.0000578	Pa×s	976.58	Joback Method
dvisc	0.0001613	Pa×s	733.99	Joback Method
hvapt	107.60	kJ/mol	418.00	NIST Webbook
psub	1.50e-05	kPa	392.81	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	4.43e-06	kPa	383.16	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.37e-06	kPa	373.17	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.29e-07	kPa	353.11	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	2.25e-08	kPa	343.44	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	4.26e-07	kPa	363.19	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68631492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures:	https://www.doi.org/10.1021/je400520e
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume