2,2',4,4',5,-Penabromodiphenyl ether

Other names:	2,2',4,4',5-Pentabromodiphenyl ether
	BDE-99
Inchi:	InChI=1S/C12H5Br5O/c13-6-1-2-11(9(16)3-6)18-12-5-8(15)7(14)4-10(12)17/h1-5H
InchiKey:	WHPVYXDFIXRKLN-UHFFFAOYSA-N
Formula:	C12H5Br5O
SMILES:	Brc1ccc(Oc2cc(Br)c(Br)cc2Br)c(Br)c1
Mol. weight [g/mol]:	564.69
CAS:	60348-60-9

Physical Properties

Property code	Value	Unit	Source
gf	193.43	kJ/mol	Joback Method
hf	124.13	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.291		Crippen Method
mcvol	225.790	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
tb	905.44	K	Joback Method
tc	1206.95	K	Joback Method
tf	661.67	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.29	J/mol×K	1056.19	Joback Method
cpg	475.69	J/mol×K	1206.95	Joback Method
cpg	469.59	J/mol×K	1156.70	Joback Method
cpg	463.50	J/mol×K	1106.44	Joback Method
cpg	436.55	J/mol×K	905.44	Joback Method
cpg	443.94	J/mol×K	955.69	Joback Method
cpg	450.81	J/mol×K	1005.94	Joback Method

dvisc	0.0001236	Pa×s	783.56	Joback Method
dvisc	0.0000884	Pa×s	864.81	Joback Method
dvisc	0.0000765	Pa×s	905.44	Joback Method
dvisc	0.0001037	Pa×s	824.18	Joback Method
dvisc	0.0002386	Pa×s	661.67	Joback Method
dvisc	0.0001868	Pa×s	702.30	Joback Method
dvisc	0.0001503	Pa×s	742.93	Joback Method
hvapt	100.30	kJ/mol	418.00	NIST Webbook
hvapt	104.80	kJ/mol	440.00	NIST Webbook
psub	4.86e-06	kPa	353.50	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.82e-06	kPa	343.46	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	5.35e-07	kPa	333.51	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.32e-07	kPa	323.60	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=C60348609&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

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