

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	Paxs	783.56	Joback Method
dvisc	0.0000884	Paxs	864.81	Joback Method
dvisc	0.0000765	Paxs	905.44	Joback Method
dvisc	0.0001037	Paxs	824.18	Joback Method
dvisc	0.0002386	Paxs	661.67	Joback Method
dvisc	0.0001868	Paxs	702.30	Joback Method
dvisc	0.0001503	Paxs	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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, Joback Method:

<https://www.doi.org/10.1021/je400520e>

1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures:

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=C60348609&Units=SI>

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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