

Dibromophenyl ether

Other names:	2,2',4,4'-Tetrabromodiphenyl ether BDE-47
Inchi:	InChI=1S/C12H6Br4O/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6H
InchiKey:	XYBSIYMGXVUUGY-UHFFFAOYSA-N
Formula:	C12H6Br4O
SMILES:	<chem>Brc1ccc(Oc2ccc(Br)cc2Br)c(Br)c1</chem>
Mol. weight [g/mol]:	485.79
CAS:	5436-43-1

Physical Properties

Property code	Value	Unit	Source
gf	188.74	kJ/mol	Joback Method
hf	109.27	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.529		Crippen Method
mvol	208.290	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	834.30	K	Joback Method
tc	1127.74	K	Joback Method
tf	589.35	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.90	J/mol×K	834.30	Joback Method
cpg	426.46	J/mol×K	883.21	Joback Method
cpg	434.25	J/mol×K	932.11	Joback Method
cpg	441.38	J/mol×K	981.02	Joback Method
cpg	447.96	J/mol×K	1029.92	Joback Method
cpg	454.12	J/mol×K	1078.83	Joback Method
cpg	459.97	J/mol×K	1127.74	Joback Method

dvisc	0.0000989	Paxs	834.30	Joback Method
dvisc	0.0002675	Paxs	630.17	Joback Method
dvisc	0.0003545	Paxs	589.35	Joback Method
dvisc	0.0001677	Paxs	711.83	Joback Method
dvisc	0.0001380	Paxs	752.65	Joback Method
dvisc	0.0001158	Paxs	793.47	Joback Method
dvisc	0.0002088	Paxs	671.00	Joback Method
psub	2.54e-07	kPa	313.54	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	9.18e-07	kPa	323.60	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	3.16e-06	kPa	333.47	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	8.63e-06	kPa	343.36	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	2.42e-05	kPa	353.37	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=C5436431&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 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

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
h vap:	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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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