3,3',4,4'-Tetrabromodiphenyl ether

Other names: PBDE Congener No. 77
Inchi: InChI=1S/C12H6Br4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H
InchiKey: RYGLOWMCGZHYRQ-UHFFFAOYSA-N
Formula: C12H6Br4O
SMILES: Brc1ccc(Oc2ccc(Br)c(Br)c2)cc1Br
Mol. weight [g/mol]: 485.79
CAS: 93703-48-1

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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.97	J/mol×K	1127.74	Joback Method
cpg	454.12	J/mol×K	1078.83	Joback Method
cpg	447.96	J/mol×K	1029.92	Joback Method
cpg	441.38	J/mol×K	981.02	Joback Method
cpg	434.25	J/mol×K	932.11	Joback Method
cpg	426.46	J/mol×K	883.21	Joback Method
cpg	417.90	J/mol×K	834.30	Joback Method
dvisc	0.0003545	Pa×s	589.35	Joback Method

dvisc	0.0000989	Pa×s	834.30	Joback Method
dvisc	0.0001158	Pa×s	793.47	Joback Method
dvisc	0.0001380	Pa×s	752.65	Joback Method
dvisc	0.0001677	Pa×s	711.83	Joback Method
dvisc	0.0002088	Pa×s	671.00	Joback Method
dvisc	0.0002675	Pa×s	630.17	Joback Method
hvapt	95.30	kJ/mol	418.00	NIST Webbook

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=C93703481&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume