Pentabromophenyl ether

Other names:

1,1'-Oxybis (2,3,4,5,6-pentabromobenzene)
6,6'-oxybis(1,2,3,4,5-pentabromobenzene)
BR 55N
Benzene, 1,1'-oxybis*2,3,4,5,6-pentabromo-
Benzene, 1,1'-oxybis[2,3,4,5,6-pentabromo-
Benzene, 1,1'-oxybis[pentabromo-
Berkflam B 10E
Bromkal 81
Bromkal 82-0DE
Bromkal 82-ode
Bromkal 83-10DE
DBDPE
DE 83R
DECA
DPBPO
Dbdpo
Decabrom
Decabromdiphenyl oxide
Decabromobiphenyl ether
Decabromobiphenyl oxide
Decabromophenyl ether
Ether, bis(pentabromophenyl)
Ether, decabromodiphenyl
F/R-P 53
FR 300
FR 300BA
FR-1210
FRP 53
Great lakes DE-83R
NCI-C55287
Octaguard FR-01
Octoguard FR-01
Pentabromodiphenyl ether
Pentabromodiphenyl ether1,1'-oxybis(2,3,4,5,6-pentabromobenzene)
Planelon DB 100
Saytex 102
Saytex 102E
Tardex 100
Themoguard 505
Thermoguard 505

	bis(pentabromophenyl) ether
	decabromodiphenyl ether
	decabromodiphenyl oxide
Inchi:	InChI=1S/C12Br10O/c13-1-3(15)7(19)11(8(20)4(1)16)23-12-9(21)5(17)2(14)6(18)10(12)2
InchiKey:	WHHGLZMJPXIBIX-UHFFFAOYSA-N
Formula:	C12Br10O
SMILES:	Brc1c(Br)c(Br)c(Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1Br
Mol. weight [g/mol]:	959.17
CAS:	1163-19-5

Physical Properties

Property code	Value	Unit	Source
gf	216.88	kJ/mol	Joback Method
hf	198.43	kJ/mol	Joback Method
hfus	65.07	kJ/mol	Joback Method
hvap	120.24	kJ/mol	Joback Method
log10ws	-14.74		Crippen Method
logp	11.104		Crippen Method
mcvol	313.290	ml/mol	McGowan Method
pc	7121.37	kPa	Joback Method
tb	1261.14	K	Joback Method
tc	1594.66	K	Joback Method
tf	1023.27	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.15	J/mol×K	1261.14	Joback Method
cpg	529.09	J/mol×K	1316.73	Joback Method
cpg	541.54	J/mol×K	1372.31	Joback Method
cpg	555.73	J/mol×K	1427.90	Joback Method
cpg	571.88	J/mol×K	1483.49	Joback Method
cpg	590.23	J/mol×K	1539.07	Joback Method
cpg	610.98	J/mol×K	1594.66	Joback Method
dvisc	0.0000342	Pa×s	1023.27	Joback Method
dvisc	0.0000296	Pa×s	1062.91	Joback Method

dvisc	0.0000259	Pa×s	1102.56	Joback Method
dvisc	0.0000228	Pa×s	1142.20	Joback Method
dvisc	0.0000203	Pa×s	1181.85	Joback Method
dvisc	0.0000182	Pa×s	1221.49	Joback Method
dvisc	0.0000165	Pa×s	1261.14	Joback Method

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=C1163195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Decabromodiphenyl Ether in Different Solvents at (283.0 to 323.0) K:	https://www.doi.org/10.1021/je100316k

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
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