

Phenol, 4,4'-(1-methylethylidene)bis[2,6-dibromo-

Other names:

2,2',6,6'-Tetrabromo-4,4'-isopropylidene bisphenol

2,2',6,6'-Tetrabromo-4,4'-isopropylidenediphenol

2,2',6,6'-Tetrabromobisphenol A

2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol

2,2-Bis(4-hydroxy-3,5-dibromophenyl)propane

2,2-bis(3,5-dibromo-4-hydroxyphenyl)propane

3,3',5,5'-Tetrabromo-4,4'-dihydroxy-2,2'-diphenylpropane

3,3',5,5'-Tetrabromobisphenol A

3,5,3',5'-Tetrabromobisphenol A

4,4'-(1-Methylethylidene)bis[2,6-dibromophenol]

4,4'-(propane-2,2-diyl)bis(2,6-dibromophenol)

4,4'-Isopropylidenebis(2,6-dibromophenol)

4,4'-Isopropylidenebis(2,6-dibromophenol)

BA 59

Bromdian

FG 2000

FR-1524

Fire Guard 2000

Firemaster BP4A

Great Lakes BA-59P

NSC 59775

Phenol, 4,4'-(2,2-propanediyl) bis[2,6-dibromo]-

Phenol, 4,4'-isopropylidenebis[2,6-dibromo-

Saytex RB 100PC

Saytex RB-100

Tetrabromobisphenol "A"

Tetrabromobisphenol A

Tetrabromodian

Tetrabromodiphenylpropane

Inchi:

InChI=1S/C15H12Br4O2/c1-15(2,7-3-9(16)13(20)10(17)4-7)8-5-11(18)14(21)12(19)6-8/h

InchiKey:

VEORPZCZECFIRK-UHFFFAOYSA-N

Formula:

C15H12Br4O2

SMILES:

CC(C)(c1cc(Br)c(O)c(Br)c1)c1cc(Br)c(O)c(Br)c1

Mol. weight [g/mol]:

543.87

CAS:

79-94-7

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|--|
| gf | 12.60 | kJ/mol | Joback Method |
| hf | -183.80 | kJ/mol | Joback Method |
| hfus | 46.42 | kJ/mol | Joback Method |
| hvap | 106.66 | kJ/mol | Joback Method |
| log10ws | -7.83 | | Crippen Method |
| logp | 6.474 | | Crippen Method |
| mcvol | 256.430 | ml/mol | McGowan Method |
| pc | 4672.09 | kPa | Joback Method |
| tb | 1038.53 | K | Joback Method |
| tc | 1336.37 | K | Joback Method |
| tf | 453.15 | K | Pyrolysis kinetics of tetrabromobisphenol a (TBBPA) and electric arc furnace dust mixtures |
| vc | 0.829 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------------|---------|-----------------|---------------|
| cpg | 638.01 | J/mol×K | 1038.53 | Joback Method |
| cpg | 654.04 | J/mol×K | 1088.17 | Joback Method |
| cpg | 671.95 | J/mol×K | 1137.81 | Joback Method |
| cpg | 692.17 | J/mol×K | 1187.45 | Joback Method |
| cpg | 715.13 | J/mol×K | 1237.09 | Joback Method |
| cpg | 741.28 | J/mol×K | 1286.73 | Joback Method |
| cpg | 771.03 | J/mol×K | 1336.37 | Joback Method |
| dvisc | 0.0000004 | Paxs | 826.79 | Joback Method |
| dvisc | 0.0000003 | Paxs | 862.08 | Joback Method |
| dvisc | 0.0000002 | Paxs | 897.37 | Joback Method |
| dvisc | 0.0000001 | Paxs | 932.66 | Joback Method |
| dvisc | 0.0000001 | Paxs | 967.95 | Joback Method |
| dvisc | 7.8338700e-08 | Paxs | 1003.24 | Joback Method |
| dvisc | 5.9764829e-08 | Paxs | 1038.53 | Joback Method |
| hfust | 29.10 | kJ/mol | 451.50 | 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=C79947&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Pyrolysis kinetics of tetrabromobisphenol a (TBBPA) and Solubility of furnace dust mixtures: <https://www.doi.org/10.1016/j.tca.2017.12.022>
2,2',6,6'-Tetrabromo-4,4'-isopropylidene Phenol in Aqueous Pollutant Solutions: <https://www.doi.org/10.1021/je400602s>

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
hfust: Enthalpy of fusion at a given temperature
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

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