

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

Other names:

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

Tetrachlorobisphenol A

Tetrachlorodian

2,2-Bis(3,5-dichloro-4-hydroxyphenyl)propane

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

2,2-Bis[3,5-dichloro-4-oxyphenyl]propane

2,2',6,6'-Tetrachlorobisphenol A

3,3',5,5'-Tetrachlorobisphenol A

3,5,3',5'-Tetrachlorobisphenol A

4,4'-Isopropylidenebis[2,6-dichlorophenol]

4,4'-Isopropylidene-2,2',6,6'-tetrachlorodiphenol

Tetrachlordian

4,4'-(1-Methylethylidene)bis(2,6-dichlorophenol)

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

NSC 18248

2,2',6,6'-tetrachloro-4,4'-isopropylidenediphenol

Inchi:

InChI=1S/C15H12Cl4O2/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:

KYPYTERUKNKOLP-UHFFFAOYSA-N

Formula:

C15H12Cl4O2

SMILES:

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

Mol. weight [g/mol]:

366.07

CAS:

79-95-8

Physical Properties

Property code	Value	Unit	Source
gf	-92.40	kJ/mol	Joback Method
hf	-352.08	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	6.037		Crippen Method
mcvol	235.390	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	392.90 ± 0.60	K	NIST Webbook
tc	1195.55	K	Joback Method
tf	707.27	K	Joback Method
vc	0.776	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.37	J/molxK	923.61	Joback Method
cpg	615.13	J/molxK	968.93	Joback Method
cpg	627.23	J/molxK	1014.26	Joback Method
cpg	639.92	J/molxK	1059.58	Joback Method
cpg	653.49	J/molxK	1104.91	Joback Method
cpg	668.22	J/molxK	1150.23	Joback Method
cpg	684.38	J/molxK	1195.55	Joback Method
dvisc	0.0000019	Paxs	707.27	Joback Method
dvisc	0.0000011	Paxs	743.33	Joback Method
dvisc	0.0000007	Paxs	779.38	Joback Method
dvisc	0.0000005	Paxs	815.44	Joback Method
dvisc	0.0000003	Paxs	851.50	Joback Method
dvisc	0.0000002	Paxs	887.55	Joback Method
dvisc	0.0000002	Paxs	923.61	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=C79958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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