

Butylated Hydroxytoluene

Other names:

1-Hydroxy-4-methyl-2,6-di-tert-butylbenzene
2,6-BIS(1,1-DIMETHYLETHYL)-4METHYLPHENOL
2,6-Bis(1,1-dimethylethyl)-4-methylphenol
2,6-Bis(tert-butyl)-4-methylphenol
2,6-Di(tert-butyl)hydroxytoluene
2,6-Di-t-butyl-4-methylphenol
2,6-Di-t-butyl-p-cresol
2,6-Di-terc.butyl-p-kresol
2,6-Di-tert-butyl-1-hydroxy-4-methyl benzene
2,6-Di-tert-butyl-4-cresol
2,6-Di-tert-butyl-4-methylphenol
2,6-Di-tert-butyl-p-cresol
2,6-Di-tert-butyl-p-methylphenol
2,6-Di-tert-butyl-para-methylphenol
2,6-di-Butyl-para-cresol
2,6-di-ter-butul-4-methyl-phenol
2,6-di-ter-butyl-4-methyl-phenol
2,6-di-tert-Butyl-methylphenol
2,6-di-tert-butyl-p-cresol (BHT)
3,5-Di-tert-butyl-4-hydroxytoluene
4-Hydroxy-3,5-di-tert-butyltoluene
4-Methyl-2,6-di-t-butyl-phenol
4-Methyl-2,6-di-terc. butylfenol
4-Methyl-2,6-di-tert-butylphenol
4-Methyl-2,6-di-tert.-butylphenol
4-Methyl-2,6-tert-butylphenol
AO 29
AO 4K
Advastab 401
Agidol
Annulex BHT
Antioxidant 29
Antioxidant 30
Antioxidant 4K
Antioxidant DBPC
Antioxidant KB
Antrancine 8
BHT
BHT (butylated hydroxytoluene)
BHT Swanox

BUKS
Bht(food grade)
Butylated hydroxyl toluene (BHT)
Butylated hydroxytoluol
Butylhydroxytoluene
CAO 1
CAO 3
Catalin Antioxydant 1
Catalin CAO-3
Chemanox 11
DBMP
DBPC
Dalpac
Dbpc(technical grade)
Deenax
Di-ter-butyl p-cresol
Di-tert-Butyl-4-methylphenol
Di-tert-Butylparamethylphenol
Di-tert-butyl-p-cresol
Di-tert-butyl-p-methylphenol
Di-tert-butylcresol
Dibunol
Dibutyl-p-cresol
Dibutylated hydroxytoluene
Dibutylcresol
Dibutylhydroxytoluene
Ergotamine, dihydro-, monomethanesulfonate (salt)
Impruvol
Ionol
Ionol (Antioxidant)
Ionol 1
Ionol BHT
Ionol CP
Ionole
Lowinox BHT
NCI-C03598
Nipanox BHT
Nonox TBC
P 21
Parabar 441
Paranox 441
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-
Phenol, 2,6-di-tert-butyl-4-methyl-

Ralox BHT
Stavox
Sumilizer BHT
Sustane
Sustane BHT
Tenamene 3
Tenox BHT
Topanol
Topanol O
Topanol OC
Vanlube PC
Vanlube PCX
Vianol
Vulkanox KB
butylated OH tolueno
o-Di-tert-butyl-p-methylphenol
p-Cresol, 2,6-di-tert-butyl-

Inchi: InChI=1S/C15H24O/c1-10-8-11(14(2,3)4)13(16)12(9-10)15(5,6)7/h8-9,16H,1-7H3
InchiKey: NLZUEZXRPGBMBCV-UHFFFAOYSA-N
Formula: C15H24O
SMILES: Cc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 220.35
CAS: 128-37-0

Physical Properties

Property code	Value	Unit	Source
chs	-8916.00	kJ/mol	NIST Webbook
gf	19.63	kJ/mol	Joback Method
hf	-296.90	kJ/mol	NIST Webbook
hfs	-410.00	kJ/mol	NIST Webbook
hfus	18.82	kJ/mol	Joback Method
hsub	117.30	kJ/mol	NIST Webbook
hsub	91.90 ± 3.20	kJ/mol	NIST Webbook
hsub	88.00 ± 0.80	kJ/mol	NIST Webbook
hsub	113.10	kJ/mol	NIST Webbook
hvap	63.01	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
log10ws	-4.12		Crippen Method
logp	4.296		Crippen Method
mcvol	204.320	ml/mol	McGowan Method

pc	2123.64	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1518.00		NIST Webbook
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rinpol	1534.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1500.00		NIST Webbook

rinpol	1501.00	NIST Webbook
rinpol	1499.00	NIST Webbook
rinpol	1497.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1533.30	NIST Webbook
rinpol	1517.50	NIST Webbook
rinpol	1514.00	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1503.90	NIST Webbook
rinpol	1513.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1494.50	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1471.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1511.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1513.00	NIST Webbook
ripol	1916.00	NIST Webbook
ripol	1870.00	NIST Webbook
ripol	1873.00	NIST Webbook
ripol	1919.00	NIST Webbook
ripol	1919.00	NIST Webbook
ripol	1870.00	NIST Webbook
ripol	1910.00	NIST Webbook
ripol	1920.00	NIST Webbook
ripol	1919.00	NIST Webbook
ripol	1902.00	NIST Webbook
ripol	1898.00	NIST Webbook
ripol	1905.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1902.00	NIST Webbook
ripol	1910.00	NIST Webbook
ripol	1910.00	NIST Webbook
ripol	1912.00	NIST Webbook
ripol	1909.00	NIST Webbook
ripol	1867.00	NIST Webbook
ripol	1911.00	NIST Webbook
ripol	1920.00	NIST Webbook

ripol	1905.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1927.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1921.00		NIST Webbook
tb	538.20	K	NIST Webbook
tc	880.13	K	Joback Method
tf	344.00 ± 0.20	K	NIST Webbook
tf	342.86 ± 0.25	K	NIST Webbook
tf	343.00 ± 0.15	K	NIST Webbook
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.55	J/mol×K	653.40	Joback Method
cpg	597.12	J/mol×K	728.98	Joback Method
cpg	654.63	J/mol×K	880.13	Joback Method
cpg	612.75	J/mol×K	766.77	Joback Method
cpg	627.45	J/mol×K	804.56	Joback Method
cpg	641.37	J/mol×K	842.35	Joback Method
cpg	580.43	J/mol×K	691.19	Joback Method
dvisc	0.0000215	Pa×s	615.64	Joback Method
dvisc	0.0000352	Pa×s	577.88	Joback Method
dvisc	0.0000618	Pa×s	540.12	Joback Method
dvisc	0.0001181	Pa×s	502.35	Joback Method
dvisc	0.0002505	Pa×s	464.59	Joback Method
dvisc	0.0000139	Pa×s	653.40	Joback Method
dvisc	0.0006069	Pa×s	426.83	Joback Method
hfust	23.85	kJ/mol	343.70	NIST Webbook
hfust	19.85	kJ/mol	341.70	NIST Webbook
hsubt	86.80 ± 0.80	kJ/mol	318.00	NIST Webbook

hsubt	87.80	kJ/mol	323.00	NIST Webbook
hvapt	61.50	kJ/mol	447.00	NIST Webbook
hvapt	87.80	kJ/mol	323.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57262e+01
Coeff. B	-4.96090e+03
Coeff. C	-9.15900e+01
Temperature range (K), min.	412.92
Temperature range (K), max.	567.92

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.61940e+02
Coeff. B	-1.50684e+04
Coeff. C	-2.09800e+01
Coeff. D	9.03774e-06
Temperature range (K), min.	344.00
Temperature range (K), max.	720.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol892.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128370&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=892

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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