Phenol, 4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)-

Other names: Phenol, 4,4'-methylenebis[2,6-di-tert-butyl-
Antioxidant E 702
Bimox M
Binox M
E 702
Ethyl 702
Etil 702
Ionox 220
Ionox 220 Antioxidant
LZ-MB 1
MB 1 (Antioxidant)
4,4'-Methylenebis[2,6-Di-tert-butylphenol]
4,4'-Dihydroxy,3,3'-5,5'-tetra-t-butyldiphenylmethane
4,4'-Methylenebis(2,6-di-t-butylphenol)
4,4'-Dihydroxy-3,5,3',5'-tetra-tert-butyldiphenylmethane
Di(4-hydroxy-3,5-di-tert-butylphenyl)methane
L 3MB1
2,2',6,6'-Tetra-tert-butyl-4,4'-methylenediphenol
NSC 30551

Inchi: InChI=1S/C29H44O2/c1-26(2,3)20-14-18(15-21(24(20)30)27(4,5)6)13-19-16-22(28(7,8)9

InchiKey: MDWVSAYEQPLWMX-UHFFFAOYSA-N

Formula: C29H44O2

SMILES: CC(C)(C)c1cc(Cc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O

Mol. weight [g/mol]: 424.66

CAS: 118-82-1

Physical Properties

Property code	Value	Unit	Source
gf	81.72	kJ/mol	Joback Method
hf	-604.33	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	108.19	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.879		Crippen Method
mcvol	383.690	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
tb	1084.52	K	Joback Method

tc	1336.33	K	Joback Method
tf	447.70 ± 0.50	K	NIST Webbook
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1546.21	J/mol×K	1336.33	Joback Method
cpg	1511.45	J/mol×K	1294.36	Joback Method
cpg	1479.18	J/mol×K	1252.39	Joback Method
cpg	1449.05	J/mol×K	1210.43	Joback Method
cpg	1420.67	J/mol×K	1168.46	Joback Method
cpg	1393.68	J/mol×K	1126.49	Joback Method
cpg	1367.71	J/mol×K	1084.52	Joback Method
dvisc	0.0000003	Pa×s	752.63	Joback Method
dvisc	7.6240209e-09	Pa×s	1084.52	Joback Method
dvisc	1.1844857e-08	Pa×s	1029.20	Joback Method
dvisc	1.9346914e-08	Pa×s	973.89	Joback Method
dvisc	3.3524046e-08	Pa×s	918.58	Joback Method
dvisc	6.2330007e-08	Pa×s	863.26	Joback Method
dvisc	0.0000001	Pa×s	807.95	Joback Method
hfust	42.97	kJ/mol	447.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	562.20	K	5.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118821&Units=SI

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume