4,4'-Methylenebis(6-tert-butyl-o-cresol)

Other names:	Phenol, 4,4'-methylenebis[2-(1,1-dimethylethyl)-6-methyl- o-Cresol, 4,4'-methylenebis[6-tert-butyl- Ethyl Antioxidant 720 4,4'-Methylenebis(2-t-butyl-6-methylphenol) 4,4'-Methylenebis(6-t-butyl-o-cresol) 4,4'-Methylenebis(2-tert-butyl-6-methylphenol) 6,6'-di-tert-butyl-4,4'-methylenedi-o-cresol
Inchi:	InChI=1S/C23H32O2/c1-14-9-16(12-18(20(14)24)22(3,4)5)11-17-10-15(2)21(25)19(13-1
InchiKey:	RKLRVTKRKFEVQG-UHFFFAOYSA-N
Formula:	C23H32O2
SMILES:	Cc1cc(Cc2cc(C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	340.50
CAS:	96-65-1

Physical Properties

Property code	Value	Unit	Source
gf	25.52	kJ/mol	Joback Method
hf	-462.99	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	97.43	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.900		Crippen Method
mcvol	299.150	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	953.70	K	Joback Method
tc	1197.24	K	Joback Method
tf	680.17	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.66	J/mol×K	953.70	Joback Method
cpg	1001.80	J/mol×K	994.29	Joback Method

cpg	1020.88	J/mol×K	1034.88	Joback Method
cpg	1040.16	J/mol×K	1075.47	Joback Method
cpg	1059.89	J/mol×K	1116.06	Joback Method
cpg	1080.31	J/mol×K	1156.65	Joback Method
cpg	1101.67	J/mol×K	1197.24	Joback Method
dvisc	0.0000016	Pa×s	680.17	Joback Method
dvisc	0.0000008	Pa×s	725.76	Joback Method
dvisc	0.0000004	Pa×s	771.35	Joback Method
dvisc	0.0000002	Pa×s	816.94	Joback Method
dvisc	0.0000001	Pa×s	862.52	Joback Method
dvisc	9.1197039e-08	Pa×s	908.11	Joback Method
dvisc	6.0346162e-08	Pa×s	953.70	Joback Method

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96651&Units=SI

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