Phenol, 2,6-bis(1,1-dimethylethyl)-4-(methoxymethyl)-

Other names: p-Cresol, 2,6-di-tert-butyl-«alpha»-methoxy-
Ethyl Antioxidant 762
Ionol 4
2,6-di-tert-Butyl-«alpha»-methoxy-para-cresol
DTB
Methyl ether of 3,5-di-tert-butyl-4-hydroxybenzene
Phenol, 2,6-di-tert-butyl-4-methoxymethyl-
2,6-Di-tert-butyl-4-methoxymethylphenol
2,6-Di-tert-butyl-«alpha»-methoxy-p-cresol
3,5-Di-tert-butyl-4-hydroxybenzyl methyl ether
4-Methoxymethyl-2,6-di-tert-butylphenol
Agidol 42
NSC 39711

Inchi: InChI=1S/C16H26O2/c1-15(2,3)12-8-11(10-18-7)9-13(14(12)17)16(4,5)6/h8-9,17H,10H2

InchiKey: SCXYLTWTWUGEAA-UHFFFAOYSA-N

Formula: C16H26O2

SMILES: COCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1

Mol. weight [g/mol]: 250.38

CAS: 87-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-76.95	kJ/mol	Joback Method
hf	-487.01	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	67.64	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	4.134		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
tb	698.70	K	Joback Method
tc	918.63	K	Joback Method
tf	374.40 ± 0.20	K	NIST Webbook
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.65	J/mol×K	698.70	Joback Method
cpg	722.49	J/mol×K	881.97	Joback Method
cpg	708.43	J/mol×K	845.32	Joback Method
cpg	693.63	J/mol×K	808.66	Joback Method
cpg	677.97	J/mol×K	772.01	Joback Method
cpg	661.35	J/mol×K	735.35	Joback Method
cpg	735.92	J/mol×K	918.63	Joback Method
dvisc	0.0000076	Pa×s	698.70	Joback Method
dvisc	0.0000115	Pa×s	658.97	Joback Method
dvisc	0.0000185	Pa×s	619.24	Joback Method
dvisc	0.0000317	Pa×s	579.52	Joback Method
dvisc	0.0000587	Pa×s	539.79	Joback Method
dvisc	0.0001202	Pa×s	500.06	Joback Method
dvisc	0.0002782	Pa×s	460.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87978&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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