3,5-di-tert-Butyl-4-hydroxybenzyl alcohol

Other names:	3,5-di-t-Butyl-4-hydroxybenzyl alcohol
	2,6-di-tert-Butyl-4-hydroxymethyl phenol
	2,6-di-t-Butyl-4-hydroxymethylphenol
	Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-
	AO 754
	Benzyl alcohol, 3,5-di-tert-butyl-4-hydroxy-
	Ionox 100
	Ionox 100 antioxidant
	Antioxidant 754
	Benzenemethanol, 4-hydroxy-3,5-di-tert-butyl
	3,5-Bis(1,1-dimethylethyl)-4-hydroxybenzenemethanol
	NSC 159133
	Benzenemethanol, 4-hydroxy-3,5-di-tert.-butyl
Inchi:	InChI=1S/C15H24O2/c1-14(2,3)11-7-10(9-16)8-12(13(11)17)15(4,5)6/h7-8,16-17H,9H2,1
InchiKey:	HNURKXXMYARGAY-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CC(C)(C)c1cc(CO)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	236.35
CAS:	88-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-117.19	kJ/mol	Joback Method
hf	-486.38	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.479		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	745.58	K	Joback Method
tc	956.84	K	Joback Method
tf	487.65	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.90	J/mol×K	745.58	Joback Method
cpg	636.26	J/mol×K	780.79	Joback Method
cpg	649.84	J/mol×K	816.00	Joback Method
cpg	662.76	J/mol×K	851.21	Joback Method
cpg	675.13	J/mol×K	886.42	Joback Method
cpg	687.06	J/mol×K	921.63	Joback Method
cpg	698.67	J/mol×K	956.84	Joback Method
dvisc	0.0001656	Pa×s	487.65	Joback Method
dvisc	0.0000575	Pa×s	530.64	Joback Method
dvisc	0.0000234	Pa×s	573.63	Joback Method
dvisc	0.0000108	Pa×s	616.62	Joback Method
dvisc	0.0000055	Pa×s	659.60	Joback Method
dvisc	0.0000031	Pa×s	702.59	Joback Method
dvisc	0.0000018	Pa×s	745.58	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=C88266&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