BENZENEMETHANOL, 3,5-BIS(1,1-DIMETHYLETHYL)-4-HYDROXY-

Other names: 2,6-di-t-Butyl-4-hydroxymethylphenol
2,6-di-tert-Butyl-4-hydroxymethyl phenol
3,5-Bis(1,1-dimethylethyl)-4-hydroxybenzenemethanol
3,5-di-t-Butyl-4-hydroxybenzyl alcohol
AO 754
Antioxidant 754
Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-
Benzenemethanol, 4-hydroxy-3,5-di-tert-butyl
Benzenemethanol, 4-hydroxy-3,5-di-tert.-butyl
Benzyl alcohol, 3,5-di-tert-butyl-4-hydroxy-
Ionox 100
Ionox 100 antioxidant
NSC 159133

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]: 236.36

Physical Properties

Property code	Value	Unit	Source
hf	-448.83	kJ/mol	Cheméo Relay (1.0)
hfus	22.91	kJ/mol	Joback Method
hvap	102.17	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
logp	3.479		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
tb	560.50	K	Cheméo Relay (1.0)
tf	394.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.90	J/mol×K	745.58	Joback Method

cpg	698.67	J/mol×K	956.84	Joback Method
cpg	687.06	J/mol×K	921.63	Joback Method
cpg	675.13	J/mol×K	886.42	Joback Method
cpg	662.76	J/mol×K	851.21	Joback Method
cpg	649.84	J/mol×K	816.00	Joback Method
cpg	636.26	J/mol×K	780.79	Joback Method
dvisc	0.0000108	Pa×s	616.62	Joback Method
dvisc	0.0000018	Pa×s	745.58	Joback Method
dvisc	0.0000031	Pa×s	702.59	Joback Method
dvisc	0.0000055	Pa×s	659.60	Joback Method
dvisc	0.0001656	Pa×s	487.65	Joback Method
dvisc	0.0000234	Pa×s	573.63	Joback Method
dvisc	0.0000575	Pa×s	530.64	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88266&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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