3,5-di-tert-Butyl-4-hydroxybenzaldehyde

Other names:	Benzaldehyde, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-
	Benzaldehyde, 3,5-di-tert-butyl-4-hydroxy-
	4-Formyl-2,6-di-tert-butylphenol
	Benzoic aldehyde, 3,5-di-t-butyl-4-hydroxy-
	Benzaldehyde, 4-hydroxy-3,5-di-tert-butyl
	Benzaldehyde, 4-hydroxy-3,5-di-tert.-butyl
	3,5-Di-tert-butyl-4-hydroxybenzadehyde
	Butylated hydroxytoluene aldehyde
Inchi:	InChI=1S/C15H22O2/c1-14(2,3)11-7-10(9-16)8-12(13(11)17)15(4,5)6/h7-9,17H,1-6H3
InchiKey:	DOZRDZLFLOODMB-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CC(C)(C)c1cc(C=O)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	234.33
CAS:	1620-98-0

Physical Properties

Property code	Value	Unit	Source
gf	-79.89	kJ/mol	Joback Method
hf	-419.73	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.800		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	702.06	K	Joback Method
tc	930.12	K	Joback Method
tf	468.83	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.56	J/mol×K	702.06	Joback Method
cpg	651.43	J/mol×K	892.11	Joback Method
cpg	638.96	J/mol×K	854.10	Joback Method
cpg	625.87	J/mol×K	816.09	Joback Method
cpg	612.03	J/mol×K	778.08	Joback Method
cpg	597.31	J/mol×K	740.07	Joback Method
cpg	663.43	J/mol×K	930.12	Joback Method
dvisc	0.0000120	Pa×s	702.06	Joback Method
dvisc	0.0000179	Pa×s	663.19	Joback Method
dvisc	0.0000282	Pa×s	624.32	Joback Method
dvisc	0.0000472	Pa×s	585.44	Joback Method
dvisc	0.0000850	Pa×s	546.57	Joback Method
dvisc	0.0001675	Pa×s	507.70	Joback Method
dvisc	0.0003692	Pa×s	468.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620980&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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume