BENZOIC ALDEHYDE, 3,5-DI-t-BUTYL-4-HYDROXY-

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]: 234.34

Physical Properties

Property code	Value	Unit	Source
hf	-398.65	kJ/mol	Cheméo Relay (1.0)
hfus	21.11	kJ/mol	Joback Method
hvap	84.95	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
logp	3.800		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	556.91	K	Cheméo Relay (1.0)
tf	377.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.56	J/mol×K	702.06	Joback Method
cpg	663.43	J/mol×K	930.12	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
dvisc	0.0000472	Pa×s	585.44	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	0.0003692	Pa×s	468.83	Joback Method
dvisc	0.0000850	Pa×s	546.57	Joback Method
dvisc	0.0001675	Pa×s	507.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620980&Units=SI
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):	

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.