Benzaldehyde, 2-hydroxy, 3,5-di(t-butyl)

Other names:	3,5-di-tert-butyl-2-hydroxybenzaldehyde
Inchi:	InChI=1S/C15H22O2/c1-14(2,3)11-7-10(9-16)13(17)12(8-11)15(4,5)6/h7-9,17H,1-6H3
InchiKey:	RRIQVLZDOZPJTH-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CC(C)(C)c1cc(C=O)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	234.33

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
рс	2276.24	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	702.06	К	Joback Method
tc	930.12	К	Joback Method
tf	468.83	К	Joback Method
VC	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.43	J/mol×K	930.12	Joback Method
cpg	597.31	J/mol×K	740.07	Joback Method
cpg	612.03	J/mol×K	778.08	Joback Method
cpg	638.96	J/mol×K	854.10	Joback Method
cpg	651.43	J/mol×K	892.11	Joback Method
cpg	625.87	J/mol×K	816.09	Joback Method
cpg	581.56	J/mol×K	702.06	Joback Method
dvisc	0.0003692	Pa×s	468.83	Joback Method

dvisc	0.0000850	Paxs	546.57 Joback Method
dvisc	0.0000472	Paxs	585.44 Joback Method
dvisc	0.0000120	Paxs	702.06 Joback Method
dvisc	0.0000282	Paxs	624.32 Joback Method
dvisc	0.0000179	Paxs	663.19 Joback Method
dvisc	0.0001675	Paxs	507.70 Joback Method
psub	6.20e-04	kPa	308.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	5.42e-04	kPa	306.37 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	5.14e-04	kPa	306.37 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	5.05e-04	kPa	306.37 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	6.73e-04	kPa	308.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	6.31e-04	kPa	308.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	3.78e-04	kPa	304.15 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	8.61e-04	kPa	310.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	8.12e-04	kPa	310.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	8.01e-04	kPa	310.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.10e-03	kPa	312.20 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.03e-03	kPa	312.20 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.01e-03	kPa	312.20 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	3.82e-04	kPa	304.15 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	4.08e-04	kPa	304.15 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.00e-04	kPa	302.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.04e-04	kPa	302.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	3.22e-04	kPa	302.18 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.34e-04	kPa	300.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	2.37e-04	kPa	300.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

psub	2.48e-04	kPa	300.17 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3.5-di.tort.butul-2-bydroxybenzaldebyde
psub	1.76e-04	kPa	298.16 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.80e-04	kPa	298.16 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.93e-04	kPa	298.16 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.40e-04	kPa	296.28 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.43e-04	kPa	296.28 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde
psub	1.51e-04	kPa	296.28 Thermodynamic study on hydroxybenzaldehyde derivatives: 3- and 4-Hydroxybenzaldehyde isomers and 3,5-di-tert-butyl-2-hydroxybenzaldehyde

Sources

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angar Hill and the second seco	https://en.wikipedia.org/wiki/Joback_method
and 9,5-09-10-10-10-20-00-00-00-00-00-00-00-00-00-00-00-00	http://link.springer.com/article/10.1007/BF02311772

Legend

срд:	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
рс:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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