Benzaldehyde, 2-hydroxy, 3-chloro, 5-(1,1,3,3-tetramethylbutyl)

Inchi: InChI=1S/C15H21ClO2/c1-14(2,3)9-15(4,5)11-6-10(8-17)13(18)12(16)7-11/h6-8,18H,9H2

InchiKey: XYQFWHMZQAOIMD-UHFFFAOYSA-N

Formula: C15H21ClO2

SMILES: CC(C)(C)CC(C)(C)c1cc(Cl)c(O)c(C=O)c1

Mol. weight [g/mol]: 268.78

Physical Properties

Property code	Value	Unit	Source
gf	-91.82	kJ/mol	Joback Method
hf	-435.47	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.572		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	739.49	K	Joback Method
tc	970.22	K	Joback Method
tf	498.75	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.46	J/mol×K	739.49	Joback Method
cpg	622.04	J/mol×K	777.94	Joback Method
cpg	635.70	J/mol×K	816.40	Joback Method
cpg	648.61	J/mol×K	854.85	Joback Method
cpg	660.90	J/mol×K	893.31	Joback Method
cpg	672.72	J/mol×K	931.76	Joback Method
cpg	684.22	J/mol×K	970.22	Joback Method
dvisc	0.0002395	Pa×s	498.75	Joback Method

dvisc	0.0001133	Pa×s	538.87	Joback Method
dvisc	0.0000595	Pa×s	579.00	Joback Method
dvisc	0.0000340	Pa×s	619.12	Joback Method
dvisc	0.0000207	Pa×s	659.24	Joback Method
dvisc	0.0000134	Pa×s	699.37	Joback Method
dvisc	0.0000091	Pa×s	739.49	Joback Method

Sources

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=R256823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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