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

Inchi: InChI=1S/C11H13ClO2/c1-11(2,3)8-4-7(6-13)10(14)9(12)5-8/h4-6,14H,1-3H3
InchiKey: WLZAKZNRJOORCP-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CC(C)(C)c1cc(Cl)c(O)c(C=O)c1
Mol. weight [g/mol]: 212.67

Physical Properties

Property code	Value	Unit	Source
gf	-128.34	kJ/mol	Joback Method
hf	-344.16	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.156		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1704.00		NIST Webbook
tb	651.20	K	Joback Method
tc	887.01	K	Joback Method
tf	451.25	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.62	J/mol×K	651.20	Joback Method
cpg	412.50	J/mol×K	690.50	Joback Method
cpg	423.53	J/mol×K	729.80	Joback Method
cpg	433.81	J/mol×K	769.11	Joback Method
cpg	443.46	J/mol×K	808.41	Joback Method
cpg	452.60	J/mol×K	847.71	Joback Method
cpg	461.33	J/mol×K	887.01	Joback Method
dvisc	0.0005256	Pa×s	451.25	Joback Method
dvisc	0.0002690	Pa×s	484.57	Joback Method

dvisc	0.0001501	Pa×s	517.90	Joback Method
dvisc	0.0000899	Pa×s	551.23	Joback Method
dvisc	0.0000570	Pa×s	584.55	Joback Method
dvisc	0.0000380	Pa×s	617.88	Joback Method
dvisc	0.0000264	Pa×s	651.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R256838&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