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

Inchi: InChI=1S/C11H14O2/c1-11(2,3)9-4-5-10(13)8(6-9)7-12/h4-7,13H,1-3H3
InchiKey: ZVCQQLGWGRTXGC-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC(C)(C)c1ccc(O)c(C=O)c1
Mol. weight [g/mol]: 178.23
CAS: 2725-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-106.78	kJ/mol	Joback Method
hf	-316.95	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	61.46	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.502		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	608.79	K	Joback Method
tc	840.49	K	Joback Method
tf	408.81	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.90	J/mol×K	608.79	Joback Method
cpg	391.12	J/mol×K	647.41	Joback Method
cpg	403.34	J/mol×K	686.02	Joback Method
cpg	414.68	J/mol×K	724.64	Joback Method
cpg	425.26	J/mol×K	763.26	Joback Method
cpg	435.17	J/mol×K	801.87	Joback Method
cpg	444.55	J/mol×K	840.49	Joback Method
dvisc	0.0011022	Pa×s	408.81	Joback Method

dvisc	0.0005012	Pa×s	442.14	Joback Method
dvisc	0.0002545	Pa×s	475.47	Joback Method
dvisc	0.0001412	Pa×s	508.80	Joback Method
dvisc	0.0000843	Pa×s	542.13	Joback Method
dvisc	0.0000534	Pa×s	575.46	Joback Method
dvisc	0.0000355	Pa×s	608.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2725533&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