Benzaldehyde, 2-hydroxy, 5-butyl

Inchi: InChI=1S/C11H14O2/c1-2-3-4-9-5-6-11(13)10(7-9)8-12/h5-8,13H,2-4H2,1H3
InchiKey: RMXFTNYYIDMHAB-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CCCCc1ccc(O)c(C=O)c1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-109.62	kJ/mol	Joback Method
hf	-308.20	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	62.75	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.547		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	612.02	K	Joback Method
tc	830.29	K	Joback Method
tf	406.39	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.37	J/mol×K	612.02	Joback Method
cpg	386.95	J/mol×K	648.40	Joback Method
cpg	398.73	J/mol×K	684.78	Joback Method
cpg	409.79	J/mol×K	721.16	Joback Method
cpg	420.21	J/mol×K	757.54	Joback Method
cpg	430.05	J/mol×K	793.91	Joback Method
cpg	439.39	J/mol×K	830.29	Joback Method
dvisc	0.0011070	Pa×s	406.39	Joback Method

dvisc	0.0005116	Pa×s	440.66	Joback Method
dvisc	0.0002643	Pa×s	474.93	Joback Method
dvisc	0.0001492	Pa×s	509.20	Joback Method
dvisc	0.0000905	Pa×s	543.48	Joback Method
dvisc	0.0000583	Pa×s	577.75	Joback Method
dvisc	0.0000394	Pa×s	612.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R256858&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

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