5-Sec-butyl-2-hydroxybenzaldehyde

Inchi: InChI=1S/C11H14O2/c1-3-8(2)9-4-5-11(13)10(6-9)7-12/h4-8,13H,3H2,1-2H3
InchiKey: KKECZRYVNIFRRC-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CCC(C)c1ccc(O)c(C=O)c1
Mol. weight [g/mol]: 178.23
CAS: 59893-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-112.06	kJ/mol	Joback Method
hf	-313.48	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	62.36	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.718		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	611.58	K	Joback Method
tc	834.42	K	Joback Method
tf	391.39	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.84	J/mol×K	611.58	Joback Method
cpg	431.69	J/mol×K	797.28	Joback Method
cpg	421.68	J/mol×K	760.14	Joback Method
cpg	411.07	J/mol×K	723.00	Joback Method
cpg	399.78	J/mol×K	685.86	Joback Method
cpg	387.73	J/mol×K	648.72	Joback Method
cpg	441.16	J/mol×K	834.42	Joback Method
dvisc	0.0000369	Pa×s	611.58	Joback Method
dvisc	0.0000564	Pa×s	574.88	Joback Method

dvisc	0.0000914	Pa×s	538.18	Joback Method
dvisc	0.0001590	Pa×s	501.49	Joback Method
dvisc	0.0003018	Pa×s	464.79	Joback Method
dvisc	0.0006395	Pa×s	428.09	Joback Method
dvisc	0.0015601	Pa×s	391.39	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C59893286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume