Benzaldehyde, 2-hydroxy-4-(1-methylethyl)-

Other names: 4-isopropyl salicylaldehyde
Inchi: InChI=1S/C10H12O2/c1-7(2)8-3-4-9(6-11)10(12)5-8/h3-7,12H,1-2H3
InchiKey: NSLDZVUVKUIYNL-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)c1ccc(C=O)c(O)c1
Mol. weight [g/mol]: 164.20
CAS: 536-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-120.48	kJ/mol	Joback Method
hf	-292.84	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	60.14	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.328		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
ripol	1940.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1941.00		NIST Webbook
tb	588.70	K	Joback Method
tc	815.79	K	Joback Method
tf	380.12	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.86	J/mol×K	588.70	Joback Method
cpg	339.96	J/mol×K	626.55	Joback Method
cpg	351.23	J/mol×K	664.40	Joback Method
cpg	361.75	J/mol×K	702.24	Joback Method
cpg	371.61	J/mol×K	740.09	Joback Method

cpg	380.87	J/mol×K	777.94	Joback Method
cpg	389.62	J/mol×K	815.79	Joback Method
dvisc	0.0018635	Pa×s	380.12	Joback Method
dvisc	0.0007755	Pa×s	414.88	Joback Method
dvisc	0.0003696	Pa×s	449.65	Joback Method
dvisc	0.0001959	Pa×s	484.41	Joback Method
dvisc	0.0001130	Pa×s	519.17	Joback Method
dvisc	0.0000699	Pa×s	553.94	Joback Method
dvisc	0.0000457	Pa×s	588.70	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=C536323&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume