

Benzaldehyde, 3-chloro-2-hydroxy-

Other names:	Benzaldehyde, 2-hydroxy, 3-chloro
Inchi:	InChI=1S/C7H5ClO2/c8-6-3-1-2-5(4-9)7(6)10/h1-4,10H
InchiKey:	DOHOPUBZLWVZMZ-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	O=Cc1cccc(Cl)c1O
Mol. weight [g/mol]:	156.57
CAS:	1927-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-155.23	kJ/mol	Joback Method
hf	-241.38	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.858		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1235.00		NIST Webbook
ripol	2066.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2082.00		NIST Webbook
tb	557.93	K	Joback Method
tc	797.69	K	Joback Method
tf	391.23	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.03	J/mol×K	557.93	Joback Method
cpg	224.89	J/mol×K	597.89	Joback Method
cpg	232.07	J/mol×K	637.85	Joback Method
cpg	238.67	J/mol×K	677.81	Joback Method
cpg	244.76	J/mol×K	717.77	Joback Method
cpg	250.42	J/mol×K	757.73	Joback Method
cpg	255.74	J/mol×K	797.69	Joback Method
dvisc	0.0013964	Pa×s	391.23	Joback Method
dvisc	0.0007298	Pa×s	419.01	Joback Method
dvisc	0.0004135	Pa×s	446.80	Joback Method
dvisc	0.0002504	Pa×s	474.58	Joback Method
dvisc	0.0001603	Pa×s	502.36	Joback Method
dvisc	0.0001075	Pa×s	530.15	Joback Method
dvisc	0.0000750	Pa×s	557.93	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1927942&Units=SI

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

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