

Benzaldehyde, 3,6-dichloro-2-hydroxy-

Other names:	Benzaldehyde, 2-hydroxy, 3,6-dichloro
Inchi:	InChI=1S/C7H4Cl2O2/c8-5-1-2-6(9)7(11)4(5)3-10/h1-3,11H
InchiKey:	JQZDVFAQNRLCDC-UHFFFAOYSA-N
Formula:	C7H4Cl2O2
SMILES:	O=Cc1c(Cl)ccc(Cl)c1O
Mol. weight [g/mol]:	191.01
CAS:	27164-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-176.79	kJ/mol	Joback Method
hf	-268.59	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.511		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
ripol	1403.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2138.00		NIST Webbook
tb	600.34	K	Joback Method
tc	844.92	K	Joback Method
tf	433.67	K	Joback Method
vc	0.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.27	J/molxK	600.34	Joback Method
cpg	263.28	J/molxK	804.16	Joback Method
cpg	258.26	J/molxK	763.39	Joback Method
cpg	252.93	J/molxK	722.63	Joback Method
cpg	247.21	J/molxK	681.87	Joback Method
cpg	241.01	J/molxK	641.10	Joback Method
cpg	268.07	J/molxK	844.92	Joback Method
dvisc	0.0000564	Paxs	600.34	Joback Method
dvisc	0.0000776	Paxs	572.56	Joback Method
dvisc	0.0001102	Paxs	544.78	Joback Method
dvisc	0.0001627	Paxs	517.00	Joback Method
dvisc	0.0002511	Paxs	489.23	Joback Method
dvisc	0.0004081	Paxs	461.45	Joback Method
dvisc	0.0007061	Paxs	433.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C27164096&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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