Benzaldehyde, 2-chloro-4-hydroxy-3,5-dimethoxy-

Other names: 1,3,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methanoisobenzofuran
Inchi: InChI=1S/C9H9ClO4/c1-13-6-3-5(4-11)7(10)9(14-2)8(6)12/h3-4,12H,1-2H3
InchiKey: GRIHRCLOUQZXPD-UHFFFAOYSA-N
Formula: C9H4Cl8O
SMILES: COc1cc(C=O)c(Cl)c(OC)c1O
Mol. weight [g/mol]: 411.75
CAS: 76341-69-0

Physical Properties

Property code	Value	Unit	Source
gf	-367.65	kJ/mol	Joback Method
hf	-570.04	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	68.83	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.875		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	658.49	K	Joback Method
tc	884.28	K	Joback Method
tf	483.27	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.38	J/mol×K	658.49	Joback Method
cpg	387.79	J/mol×K	846.65	Joback Method
cpg	380.24	J/mol×K	809.02	Joback Method
cpg	372.25	J/mol×K	771.39	Joback Method
cpg	363.79	J/mol×K	733.75	Joback Method
cpg	354.84	J/mol×K	696.12	Joback Method
cpg	394.91	J/mol×K	884.28	Joback Method
dvisc	0.0000225	Pa×s	658.49	Joback Method

dvisc	0.0000302	Pa×s	629.29	Joback Method
dvisc	0.0000416	Pa×s	600.08	Joback Method
dvisc	0.0000593	Pa×s	570.88	Joback Method
dvisc	0.0000878	Pa×s	541.68	Joback Method
dvisc	0.0001361	Pa×s	512.47	Joback Method
dvisc	0.0002222	Pa×s	483.27	Joback Method

Sources

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=C76341690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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