Benzaldehyde, 4-chloro-

Other names:	Benzaldehyde, p-chloro-
	p-Chlorobenzaldehyde
	4-Chlorobenzaldehyde
	p-Chlorobenzenecarboxaldehyde
	4-Chlorbenzaldehyd
Inchi:	InChI=1S/C7H5ClO/c8-7-3-1-6(5-9)2-4-7/h1-5H
InchiKey:	AVPYQKSLYISFPO-UHFFFAOYSA-N
Formula:	C7H5ClO
SMILES:	O=Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	140.57
CAS:	104-88-1

Physical Properties

Property code	Value	Unit	Source
affp	831.30	kJ/mol	NIST Webbook
basg	799.40	kJ/mol	NIST Webbook
chs	-3346.40 ± 8.40	kJ/mol	NIST Webbook
ea	0.68 ± 0.09	eV	NIST Webbook
ea	0.66 ± 0.09	eV	NIST Webbook
gf	-0.61	kJ/mol	Joback Method
hf	-64.07	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
ie	9.61 ± 0.01	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.59	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	2.152		Crippen Method
mcvol	99.540	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1113.20		NIST Webbook
rinpol	1122.60		NIST Webbook
tb	486.70	K	NIST Webbook
tc	704.10	K	Joback Method

tf	319.85 ± 1.00	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.88	J/mol×K	477.31	Joback Method
cpg	217.17	J/mol×K	666.30	Joback Method
cpg	210.42	J/mol×K	628.50	Joback Method
cpg	203.14	J/mol×K	590.70	Joback Method
cpg	195.31	J/mol×K	552.91	Joback Method
cpg	186.90	J/mol×K	515.11	Joback Method
cpg	223.42	J/mol×K	704.10	Joback Method
dvisc	0.0003318	Pa×s	477.31	Joback Method
dvisc	0.0004071	Pa×s	444.34	Joback Method
dvisc	0.0005162	Pa×s	411.38	Joback Method
dvisc	0.0006820	Pa×s	378.41	Joback Method
dvisc	0.0009504	Pa×s	345.44	Joback Method
dvisc	0.0014204	Pa×s	312.48	Joback Method
dvisc	0.0023338	Pa×s	279.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104881&Units=SI

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

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume