

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	0.66 ± 0.09	eV	NIST Webbook
ea	0.68 ± 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	9.57	eV	NIST Webbook
ie	9.59	eV	NIST Webbook
ie	9.61 ± 0.01	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

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

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=C104881&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	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

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