Benzaldehyde, 2-chloro-

Other names:	2-Chlorbenzaldehyd
	2-Chlorobenzaldehyde
	2-Clorobenzaldeide
	Benzaldehyde, o-chloro-
	NSC 15347
	USAF M-7
	o-Chloorbenzaldehyde
	o-Chlorobenzaldehyde
	o-Chlorobenzenecarboxaldehyde
	o-Chloroformylbenzene
Inchi:	InChI=1S/C7H5ClO/c8-7-4-2-1-3-6(7)5-9/h1-5H
InchiKey:	FPYUJUBAXZAQNL-UHFFFAOYSA-N
Formula:	C7H5ClO
SMILES:	O=Cc1ccccc1Cl
Mol. weight [g/mol]:	140.57
CAS:	89-98-5

Physical Properties

Property code	Value	Unit	Source
chl	-3374.40 ± 8.40	kJ/mol	NIST Webbook
chl	-3372.00	kJ/mol	NIST Webbook
gf	-0.61	kJ/mol	Joback Method
hf	-64.07	kJ/mol	Joback Method
hfl	-98.00	kJ/mol	NIST Webbook
hfus	14.02	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.152		Crippen Method
mcvol	99.540	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1112.70		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1122.40		NIST Webbook
rinpol	1106.00		NIST Webbook
tb	485.19 ± 0.07	K	NIST Webbook
tb	485.10	K	NIST Webbook

tc	704.10	K	Joback Method
tf	284.80 ± 0.05	K	NIST Webbook
tf	285.30 ± 0.02	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.42	J/mol×K	704.10	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	177.88	J/mol×K	477.31	Joback Method
dvisc	0.0023338	Pa×s	279.51	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
hvapt	49.80	kJ/mol	472.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70426e+01
Coeff. B	-4.81693e+03
Coeff. C	-7.41500e+01
Temperature range (K), min.	361.64
Temperature range (K), max.	484.76

Sources

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=C89985&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume