Benzaldehyde, 3-chloro-

Other names:	Benzaldehyde, m-chloro- m-Chlorobenzaldehyde meta-Chlorobenzaldehyde 3-Chlorobenzaldehyde
Inchi:	InChI=1S/C7H5ClO/c8-7-3-1-2-6(4-7)5-9/h1-5H
InchiKey:	SRWILAKSARHZPR-UHFFFAOYSA-N
Formula:	C7H5ClO
SMILES:	O=Cc1cccc(Cl)c1
Mol. weight [g/mol]:	140.57
CAS:	587-04-2

Physical Properties

Property code	Value	Unit	Source
affp	813.00	kJ/mol	NIST Webbook
basg	781.10	kJ/mol	NIST Webbook
chl	-3366.90 ± 8.40	kJ/mol	NIST Webbook
chl	-3365.00	kJ/mol	NIST Webbook
ea	0.71 ± 0.09	eV	NIST Webbook
ea	0.67 ± 0.09	eV	NIST Webbook
gf	-0.61	kJ/mol	Joback Method
hf	-64.07	kJ/mol	Joback Method
hfl	-105.00	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	1118.90		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1108.40		NIST Webbook
tb	486.70	K	NIST Webbook
tc	704.10	K	Joback Method
tf	279.51	K	Joback Method
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

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C587042&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid 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

hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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