Benzaldehyde, 2,4-dichloro-

Other names: 2,4-Dichlorobenzaldehyde
Inchi: InChI=1S/C7H4Cl2O/c8-6-2-1-5(4-10)7(9)3-6/h1-4H
InchiKey: YSFBEAASFUWWHU-UHFFFAOYSA-N
Formula: C7H4Cl2O
SMILES: O=Cc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 175.01
CAS: 874-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-22.17	kJ/mol	Joback Method
hf	-91.28	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Heat capacity and thermodynamic properties of 2,4-dichlorobenzaldehyde (C7H4Cl2O)
hvap	50.27	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.806		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	506.20	K	NIST Webbook
tc	753.22	K	Joback Method
tf	345.00 ± 4.00	K	NIST Webbook
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.00	J/mol×K	753.22	Joback Method
cpg	198.12	J/mol×K	519.72	Joback Method
cpg	206.07	J/mol×K	558.64	Joback Method
cpg	213.46	J/mol×K	597.55	Joback Method
cpg	220.33	J/mol×K	636.47	Joback Method

cpg	226.69	J/mol×K	675.39	Joback Method
cpg	232.58	J/mol×K	714.30	Joback Method
dvisc	0.0003403	Pa×s	519.72	Joback Method
dvisc	0.0018573	Pa×s	321.95	Joback Method
dvisc	0.0012274	Pa×s	354.91	Joback Method
dvisc	0.0008704	Pa×s	387.87	Joback Method
dvisc	0.0006513	Pa×s	420.84	Joback Method
dvisc	0.0005084	Pa×s	453.80	Joback Method
dvisc	0.0004103	Pa×s	486.76	Joback Method
hfust	20.47	kJ/mol	347.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat capacity and thermodynamic properties of 2,4-dichlorobenzaldehyde (C7H4Cl2O):	https://www.doi.org/10.1016/j.jct.2004.01.006
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=C874420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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