

2,3-Dichlorobenzaldehyde

Other names:	Benzaldehyde, 2,3-dichloro-
Inchi:	InChI=1S/C7H4Cl2O/c8-6-3-1-2-5(4-10)7(6)9/h1-4H
InchiKey:	LLMLNAVBOAMOE-UEHFFFAOYSA-N
Formula:	C7H4Cl2O
SMILES:	O=Cc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	175.01
CAS:	6334-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-22.17	kJ/mol	Joback Method
hf	-91.28	kJ/mol	Joback Method
hfus	17.83	kJ/mol	Joback Method
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
rinpol	1279.00		NIST Webbook
tb	519.72	K	Joback Method
tc	753.22	K	Joback Method
tf	321.95	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	238.00	J/mol×K	753.22	Joback Method

dvisc	0.0018573	Paxs	321.95	Joback Method
dvisc	0.0012274	Paxs	354.91	Joback Method
dvisc	0.0008704	Paxs	387.87	Joback Method
dvisc	0.0006513	Paxs	420.84	Joback Method
dvisc	0.0005084	Paxs	453.80	Joback Method
dvisc	0.0004103	Paxs	486.76	Joback Method
dvisc	0.0003403	Paxs	519.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6334185&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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