2,3,6-Trichlorobenzaldehyde

Other names: Benzaldehyde, 2,3,6-trichloro-
Inchi: InChI=1S/C7H3Cl3O/c8-5-1-2-6(9)7(10)4(5)3-11/h1-3H
InchiKey: AURSMWWOMOVHBM-UHFFFAOYSA-N
Formula: C7H3Cl3O
SMILES: O=Cc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 209.46
CAS: 4659-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-43.73	kJ/mol	Joback Method
hf	-118.49	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.459		Crippen Method
mcvol	124.020	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	562.13	K	Joback Method
tc	801.27	K	Joback Method
tf	364.39	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.23	J/mol×K	562.13	Joback Method
cpg	223.17	J/mol×K	601.99	Joback Method
cpg	229.61	J/mol×K	641.84	Joback Method
cpg	235.58	J/mol×K	681.70	Joback Method
cpg	241.09	J/mol×K	721.56	Joback Method
cpg	246.17	J/mol×K	761.42	Joback Method
cpg	250.83	J/mol×K	801.27	Joback Method
dvisc	0.0015051	Pa×s	364.39	Joback Method

dvisc	0.0010563	Pa×s	397.35	Joback Method
dvisc	0.0007826	Pa×s	430.30	Joback Method
dvisc	0.0006051	Pa×s	463.26	Joback Method
dvisc	0.0004841	Pa×s	496.22	Joback Method
dvisc	0.0003982	Pa×s	529.17	Joback Method
dvisc	0.0003352	Pa×s	562.13	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=C4659476&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume