Benzaldehyde, 4,5,6-trichloro-2-hydroxy

Inchi: InChI=1S/C7H3Cl3O2/c8-4-1-5(12)3(2-11)6(9)7(4)10/h1-2,12H
InchiKey: DSYXJIUEIAOOAD-UHFFFAOYSA-N
Formula: C7H3Cl3O2
SMILES: O=Cc1c(O)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 225.46

Physical Properties

Property code	Value	Unit	Source
gf	-198.35	kJ/mol	Joback Method
hf	-295.80	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.165		Crippen Method
mcvol	129.890	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	642.75	K	Joback Method
tc	891.37	K	Joback Method
tf	476.11	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	249.64	J/mol×K	642.75	Joback Method
cpg	274.98	J/mol×K	849.94	Joback Method
cpg	270.47	J/mol×K	808.50	Joback Method
cpg	265.76	J/mol×K	767.06	Joback Method
cpg	260.77	J/mol×K	725.62	Joback Method
cpg	255.42	J/mol×K	684.19	Joback Method
cpg	279.36	J/mol×K	891.37	Joback Method
dvisc	0.0000425	Pa×s	642.75	Joback Method
dvisc	0.0000566	Pa×s	614.98	Joback Method
dvisc	0.0000774	Pa×s	587.20	Joback Method
dvisc	0.0001092	Pa×s	559.43	Joback Method
dvisc	0.0001597	Pa×s	531.66	Joback Method
dvisc	0.0002435	Pa×s	503.88	Joback Method
dvisc	0.0003900	Pa×s	476.11	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=R45596&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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume