Benzaldehyde, 2,5-dichloro-4-hydroxy

Inchi: InChI=1S/C7H4Cl2O2/c8-5-2-7(11)6(9)1-4(5)3-10/h1-3,11H
InchiKey: BUJHRHRKNMSZAW-UHFFFAOYSA-N
Formula: C7H4Cl2O2
SMILES: O=Cc1cc(Cl)c(O)cc1Cl
Mol. weight [g/mol]: 191.01

Physical Properties

Property code	Value	Unit	Source
gf	-176.79	kJ/mol	Joback Method
hf	-268.59	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.511		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	600.34	K	Joback Method
tc	844.92	K	Joback Method
tf	433.67	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.27	J/mol×K	600.34	Joback Method
cpg	241.01	J/mol×K	641.10	Joback Method

cpg	247.21	J/mol×K	681.87	Joback Method
cpg	252.93	J/mol×K	722.63	Joback Method
cpg	258.26	J/mol×K	763.39	Joback Method
cpg	263.28	J/mol×K	804.16	Joback Method
cpg	268.07	J/mol×K	844.92	Joback Method
dvisc	0.0007061	Pa×s	433.67	Joback Method
dvisc	0.0004081	Pa×s	461.45	Joback Method
dvisc	0.0002511	Pa×s	489.23	Joback Method
dvisc	0.0001627	Pa×s	517.00	Joback Method
dvisc	0.0001102	Pa×s	544.78	Joback Method
dvisc	0.0000776	Pa×s	572.56	Joback Method
dvisc	0.0000564	Pa×s	600.34	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=R45528&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