tetrachloro-4-hydroxybenzaldehyde

Other names: Benzaldehyde, 4-hydroxy, tetrachloro
Inchi: InChI=1S/C7H2Cl4O2/c8-3-2(1-12)4(9)6(11)7(13)5(3)10/h1,13H
InchiKey: ZIRMLCYOVCHSCE-UHFFFAOYSA-N
Formula: C7H2Cl4O2
SMILES: O=Cc1c(Cl)c(Cl)c(O)c(Cl)c1Cl
Mol. weight [g/mol]: 259.90

Physical Properties

Property code	Value	Unit	Source
gf	-219.91	kJ/mol	Joback Method
hf	-323.01	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.818		Crippen Method
mcvol	142.130	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1839.00		NIST Webbook
tb	685.16	K	Joback Method
tc	937.20	K	Joback Method
tf	518.55	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.41	J/mol×K	685.16	Joback Method

cpg	268.37	J/mol×K	727.17	Joback Method
cpg	273.02	J/mol×K	769.17	Joback Method
cpg	277.41	J/mol×K	811.18	Joback Method
cpg	281.63	J/mol×K	853.18	Joback Method
cpg	285.75	J/mol×K	895.19	Joback Method
cpg	289.84	J/mol×K	937.20	Joback Method
dvisc	0.0002305	Pa×s	518.55	Joback Method
dvisc	0.0001529	Pa×s	546.32	Joback Method
dvisc	0.0001055	Pa×s	574.09	Joback Method
dvisc	0.0000754	Pa×s	601.86	Joback Method
dvisc	0.0000554	Pa×s	629.62	Joback Method
dvisc	0.0000419	Pa×s	657.39	Joback Method
dvisc	0.0000323	Pa×s	685.16	Joback Method

Sources

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=R45621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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