Benzaldehyde, 4-hydroxy-2,3,6-trichloro

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

Physical Properties

Property code	Value	Unit	Source
hfus	27.42	kJ/mol	Joback Method
log10ws	-3.02		Cheméo Relay (1.0)
logp	3.165		Crippen Method
mcvol	129.890	ml/mol	McGowan Method
rinpol	1675.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
tf	387.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.64	J/mol×K	642.75	Joback Method
cpg	255.42	J/mol×K	684.19	Joback Method
cpg	260.77	J/mol×K	725.62	Joback Method
cpg	265.76	J/mol×K	767.06	Joback Method
cpg	270.47	J/mol×K	808.50	Joback Method
cpg	274.98	J/mol×K	849.94	Joback Method
cpg	279.36	J/mol×K	891.37	Joback Method

dvisc	0.0003900	Pa×s	476.11	Joback Method
dvisc	0.0002435	Pa×s	503.88	Joback Method
dvisc	0.0001597	Pa×s	531.66	Joback Method
dvisc	0.0001092	Pa×s	559.43	Joback Method
dvisc	0.0000774	Pa×s	587.20	Joback Method
dvisc	0.0000566	Pa×s	614.98	Joback Method
dvisc	0.0000425	Pa×s	642.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R45500&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point