2,3,6-trichloro-4-hydroxybenzaldehyde

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
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	1651.00		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
rinpol	1664.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1672.00		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	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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R45500&Units=SI
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

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