5-Chlorovanillin

Other names:	Benzaldehyde, 3-chloro-4-hydroxy-5-methoxy- Vanillin, 5-chloro- 3-chlorovanillin 5-Chloro-4-hydroxy-3-methoxybenzaldehyde
Inchi:	InChI=1S/C8H7ClO3/c1-12-7-3-5(4-10)2-6(9)8(7)11/h2-4,11H,1H3
InchiKey:	ONIVKFDMLVBDRK-UHFFFAOYSA-N
Formula:	C8H7ClO3
SMILES:	COc1cc(C=O)cc(Cl)c1O
Mol. weight [g/mol]:	186.59
CAS:	19463-48-0

Physical Properties

Property code	Value	Unit	Source
gf	-261.44	kJ/mol	Joback Method
hf	-405.71	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.867		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	608.21	K	Joback Method
tc	840.75	K	Joback Method
tf	437.25	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.34	J/mol×K	608.21	Joback Method
cpg	288.00	J/mol×K	646.97	Joback Method
cpg	296.10	J/mol×K	685.72	Joback Method
cpg	303.68	J/mol×K	724.48	Joback Method
cpg	310.82	J/mol×K	763.24	Joback Method

cpg	317.54	J/mol×K	801.99	Joback Method
cpg	323.91	J/mol×K	840.75	Joback Method
dvisc	0.0005303	Pa×s	437.25	Joback Method
dvisc	0.0003033	Pa×s	465.74	Joback Method
dvisc	0.0001850	Pa×s	494.24	Joback Method
dvisc	0.0001191	Pa×s	522.73	Joback Method
dvisc	0.0000802	Pa×s	551.22	Joback Method
dvisc	0.0000562	Pa×s	579.72	Joback Method
dvisc	0.0000407	Pa×s	608.21	Joback Method
hfust	39.40	kJ/mol	442.60	NIST Webbook

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=C19463480&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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: